ASYMPTOTIC ESTIMATES OF THE ERRORS IN THE NUMERICAL INTEGRATION OF ANALYTIC FUNCTIONS

by

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Except as stated herein this thesis contains no material which has been accepted for the award of any other degree or diploma in any University, and that, to the best of my knowledge and belief this thesis contains no copy or paraphrase of material previously published or written by another person, except when due reference is made in the text.

John D Donaldson

(John D. Donaldson)

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PREFACE

An expression in terms of a contour integral for the remainder term in a numerical integration formula of a general type is obtained. Because the function whose integral is under consideration is allowed to have singularities at the end points of the interval of integration special emphasis is placed on the behaviour of the contour at these points. It is then shown how the corresponding contour integral form of the remainder term in some of the well-known integration formulae may be derived.

The contour integral in conjunction with known asymptotic expressions for part of the integrand is used firstly to examine the convergence properties of certain quadrature schemes (Chapter III) and secondly to estimate the error in approximating to a real integral by a quadrature sum (Chapter IV).

In conclusion (Chapter V) we discuss some of the problems which are to be subjects of further research.

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CHAPTER 0

INTRODUCTION

0.1 Introduction

In this thesis we shall be concerned with the remainder when a definite integral

(0.1.1) $$I = \int_a^b \omega(x) f(x)\, dx$$

is evaluated numerically by means of a weighted sum of ordinates of the function $f(x)$. The function $\omega(x)$ is known as the weight function and is usually integrable over the real interval $[a, b]$ which is not necessarily finite; $\omega(x)$ may have singularities at the end points a, b.

The general numerical integration formula may be written

(0.1.2) $$\int_a^b \omega(x) f(x)\, dx = \sum_{k=0}^{n} \lambda_{k,n} f(x_{k,n}) + R_{n+1}(f)$$

where $R_{n+1}(f)$ is the remainder term of the formula. (The significance of the suffix $n+1$ is that the sum on the right of equation (0.1.2) contains $(n+1)$ terms; n may be infinite in which case we shall denote the remainder term by $R(f)$.) The abscissae, $x_{k,n}$, $k=0(1)n$, are points of $[a, b]$ and the coefficients, $\lambda_{k,n}$, $k=0(1)n$, are known as weight factors.

We shall also consider, but to a lesser extent, integration formulae of osculatory type. Osculatory quadrature formulae not only make use of the function values at the abscissae but also of values of the successive derivatives of the function. The formula may be written generally

$$\int_a^b \omega(x) f(x)\, dx = \sum_{r=0}^{p-1} \sum_{k=0}^{n} \lambda_{k,r,n} f^{(r)}(x_{k,n}) + R_{(n+1)p}(f). \tag{0.1.3}$$

Our aim is to find asymptotic estimates of the remainder, $R_{n+1}(f)$, for large values of n , when $f(z)$ admits of analytic continuation into a suitable region of the plane of the complex variable z , where $z = x + iy$.

The most common form of the remainder in quadrature rules is in terms of a high order derivative of the function $f(x)$, see e.g. Hildebrand [1, Chapt. 8] . This form has, however, obvious disadvantages, see Hamming [2, sect. 8.7] .

The computation of a high order derivative even for an innocent looking function like $1/(1+x^2)$ can become very tedious or sufficient information about such high order derivatives may not be readily available.

Hamming [2] points out that for many functions, e.g. $f(x) = 1/x$, the nth derivative behaves as $n!$. So that expressions in terms of derivatives for the remainder need not necessarily tend to zero for large values of n.

In most cases the object is to place an upper bound on the derivative of the function over the range of integration. That this is not always possible is obvious.

For example if we choose to integrate $x^{1/2}$ over the interval $[0,1]$ then we certainly cannot place an upper bound on the derivative of $x^{1/2}$ in $[0,1]$. One can however overcome this difficulty by choosing a formulae which "divides out" the singularity. Navot [3] has developed a formula of Euler-MacLaurin type to handle such a singularity while a formula corresponding to Simpson's is discussed by Noble [4, p.240].

On the other hand the direct application of quadrature rules to functions with algebraic and logarithmic singularities in the range of integration is considered by Ninham and Lyness [5]. Ninham and Lyness use a Fourier series representation for the function and obtain an expression for the remainder term in a general quadrature rule in terms of an infinite sum of Fourier transforms. This approach is well suited to the repeated trapezoidal rule or, like Romberg integration, a linear combination of such rules. It is not however as readily applicable to Gauss type formulae; in fact Ninham says that this process "leads to a strong preference for trapezoidal rules over the Gauss-Legendre and similar rules". Ninham is however mainly concerned with using the error expression as a correction to the quadrature sum. The results are then extended using the theory of generalised functions, see, e.g. Lighthill [6]. Ninham's analysis is not as powerful when the function to be integrated has singularities just off the interval of integration. Furthermore it cannot be applied to functions with essential singularities at the end point of the range.

There are other expressions in terms of functions of a real variable for the remainder term: there is for example an expression in terms of a real integral, see Hildebrand [1, p.165]. We shall however be concerned with methods which use complex variable techniques. Stroud [7] in his excellent bibliography on numerical integration unfortunately makes very little mention of techniques for finding the remainder term using complex variable techniques.

Two separate techniques have however come to the fore. One expresses the remainder term as a linear functional on $f(x)$ and was initiated by Davis [8]. This linear functional approach was not confined to integration formulae but was also used for differentiation and interpolation formulae. The other considers an expression for the remainder in terms of a contour integral and is probably of classical origin.

0.2 The Linear Functional Approach

The ideas put forward by Davis [8] were extended more fully with special emphasis on integration formulae by Davis and Rabinowitz [9]. There are two concepts in this paper which we make use of later in the thesis.

Davis and Rabinowitz [9] consider the remainder as a linear functional on $f(x)$, i.e.,

$$(0.2.1) \qquad R_{n+1}(f) = \int_{-1}^{+1} f(x)\,dx - \sum_{k=0}^{n} a_k f(x_k)$$

where the weight function $\omega(x) = 1$ and the interval is $[-1, 1]$. Let $z = x + iy$ be a complex variable and let $f(z)$ be the analytic continuation of $f(x)$ into the plane of z. Supposing that $f(z)$ has no singularities on $[-1, 1]$ then $f(z)$ is analytic in a region of the complex plane which has the real interval $[-1, 1]$ in its interior.

Further let us denote by $\mathcal{E}_\rho,\ \rho \geq 1$, the family of confocal ellipses with foci $-1, 1$. When $\rho = 1$, $\mathcal{E}_\rho$ corresponds to the degenerate ellipse $-1 \leq \mathcal{Re}(z) \leq 1$. The family may also be represented by $|z + (z^2-1)^{1/2}| = \rho \geq 1$. We use this family of ellipses in Chapters III and IV.

The functions $\zeta_\nu(z,\rho),\ \nu = 0, 1, 2, \ldots$, defined by

$$(0.2.2) \qquad \zeta_\nu(z,\rho) = \eta(\rho)\, U_\nu(z),$$

where $U_\nu(z)$ is the Chebyshev polynomial of the second kind and $\eta(\rho)$ is a suitable function of ρ are a complete orthonormal set for the region of the complex plane bounded by $\mathcal{E}_\rho$. Davis expands $f(z)$ in terms of the functions $\zeta_\nu(z,\rho)$ as

$$(0.2.3) \qquad f(z) = \sum_{\nu=0}^{\infty} a_\nu \zeta_\nu(z,\rho)$$

where, since $f(z)$ is analytic in the interior of $\mathcal{E}_\rho$ for some value of ρ,

$$(0.2.4) \qquad \sum_{\nu=0}^{\infty} |a_\nu|^2 = \|f\|^2 < \infty .$$

From equation (0.2.3) we thus have

$$(0.2.5) \qquad R_{n+1}(f) = \sum_{\nu=0}^{\infty} a_\nu R_{n+1}[\zeta_\nu(z,\rho)] .$$

Using Schwarz's inequality, equation (0.2.5) becomes

$$(0.2.6) \qquad |R_{n+1}(f)|^2 \leq \sum_{\nu=0}^{\infty} |a_\nu|^2 \cdot \sum_{\nu=0}^{\infty} |R_{n+1}[\zeta_\nu(z,\rho)]|^2 .$$

The expression σ_ρ^2, defined by

$$(0.2.7) \qquad \sigma_\rho^2 = \sum_{\nu=0}^{\infty} |R_{n+1}[\zeta_\nu(z,\rho)]|^2 ,$$

may be computed for several quadrature rules and values of ρ

To help us find M_ρ we can perhaps make use of the Maximum Modulus principle. For, $f(z)$ is analytic on and within $\mathcal{E}_\rho$ and the principle tells us that $|f(z)|$ takes its maximum value <u>on</u> $\mathcal{E}_\rho$.

It is found that as we let ρ increase $\|f(z)\|_{\mathcal{E}_\rho}$ will increase while σ_ρ will decrease. The value of ρ for which the product $\sigma_\rho \cdot \|f\|_{\mathcal{E}_\rho}$ is a minimum will provide the lowest upper bound of the modulus of the remainder, $R_{n+1}(f)$. In practice the value of ρ is selected from a comparison of a finite number of values of $\sigma_\rho \cdot \|f\|_{\mathcal{E}_\rho}$.

We refer to this minimising technique frequently in Chapter IV.

The linear functional approach was used by Hammerlin [11] with special regard to formulae in which the abscissae were equally spaced in the interval. Hammerlin assumed that $f(z)$ was analytic on and within the unit circle which we denote by Γ. The interval of integration was restricted to values a, b such that $-1 < a \leq b < 1$ and the remainder term was considered in the form

(0.2.10) $$R_{n+1}(f) = \int_a^b f(x)\,dx - \sum_{j=0}^{n} g_j f(x_j) .$$

From Cauchy's formula we have, since $f(z)$ is analytic on and within Γ,

(0.2.11) $$f(z) = \frac{1}{2\pi i}\int_\Gamma \frac{f(\zeta)\,d\zeta}{\zeta - z} = \frac{1}{2\pi}\int_\Gamma \frac{f(\zeta)\,ds}{1 - z\bar{\zeta}}$$

where S is the arc length on the unit circle.

From equation (0.2.11) we have

$$R_{n+1}(f) = \frac{1}{2\pi}\int_{\Gamma} R_{n+1}\left(\frac{1}{1-x\bar{\zeta}}\right) f(\zeta)\, ds \quad . \tag{0.2.12}$$

Using Schwarz's inequality we have from equation (0.2.12)

$$|R_{n+1}(f)|^2 \le \frac{1}{4\pi^2}\int_{\Gamma} \left|R_{n+1}\left(\frac{1}{1-x\bar{\zeta}}\right)\right|^2 ds \cdot \int_{\Gamma} |f(\zeta)|^2 ds \tag{0.2.13}$$

or,

$$|R_{n+1}(f)|^2 \le \sigma^2 \; \|f\|^2 \tag{0.2.14}$$

where $\|f\|$ is the norm of $f(z)$ on the unit circle.

The remaining part of Hammerlin's paper is mainly devoted to finding estimates of σ^2 for a few of the well-known rules. The method is as follows. We have

$$R_{n+1}\left(\frac{1}{1-x\bar{\zeta}}\right) = \sum_{\nu=0}^{\infty} R_{n+1}(x^{\nu}) \cdot \bar{\zeta}^{\nu} \quad . \tag{0.2.15}$$

Since $\zeta^{\nu}/(2\pi)^{1/2}$, $\nu = 0, 1, 2, \ldots$ form a complete orthonormal set of functions for Γ we have on substituting equation (0.2.15) into the expression for σ^2

$$
(0.2.16) \quad \begin{cases} \sigma^2 = \dfrac{1}{4\pi^2} \displaystyle\int_{\Gamma} \left| R_{n+1}\left(\frac{1}{1-x\bar{\xi}}\right)\right|^2 ds \\ \quad\;\; = \dfrac{1}{2\pi} \displaystyle\sum_{\nu=0}^{\infty} \left| R_{n+1}\,(x^{\nu})\right|^2 . \end{cases}
$$

To evaluate σ^2 is then only a matter of finding an expression for the remainder when the function to be integrated is a positive integral power of x. Hammerlin uses well-known expressions in terms of Bernoulli polynomials, see, e.g., Krylov [12], to place an upper bound on $|R_{n+1}(x^{\nu})|$. Upper bounds for $\sum_{\nu=0}^{\infty} |R_{n+1}(x^{\nu})|^2$ are then readily available.

An upper bound for $\|f\|$ is obtained using Schwarz's inequality. We have

$$
(0.2.17) \qquad \|f\|^2 = \int_{|z|=1} |f(z)|^2 ds \leq 2\pi \max_{z\in\Gamma} |f(z)|^2 .
$$

From equations (0.2.16) and (0.2.17) we have

$$
(0.2.18) \qquad |R_{n+1}(f)| \leq (2\pi)^{1/2}\,\sigma \cdot \max_{z\in\Gamma} |f(z)| .
$$

Values of $(2\pi)^{1/2}\cdot\sigma$ are given for a few of the well-known quadrature rules, e.g. the Trapezoidal Rule and Simpson's Rule.

The approach used by Hammerlin is generalised somewhat by himself in a following paper [13] . In this paper the function $f(z)$ is supposed analytic within and on a circle of radius r, $r > 1$, denoted by Γ_r , and integrals over the interval $[-1, 1]$ are considered.

The complete orthonormal set of functions for Γ_r are $z^\nu/[(2\pi r)^{1/2} \cdot r^\nu]$, $\nu = 0, 1, 2, \ldots$ So that if we follow the same process as in [11] we find

(0.2.19) $$|R_{n+1} f| \leq \sigma(r) \cdot \|f\|_{\Gamma_r}$$

where

(0.2.20) $$\begin{cases} \|f\|^2_{\Gamma_r} = \int_{\Gamma_r} |f(z)|^2 ds \\ \qquad = 2\pi r \sum_{\nu=0}^{\infty} a_\nu^2 \cdot r^{2\nu} \end{cases}$$

and

(0.2.21) $$\sigma^2(r) = \frac{1}{2\pi r} \sum_{\nu=0}^{\infty} \frac{|R_{n+1}(x^\nu)|^2}{r^{2\nu}} .$$

Hammerlin again uses expressions for the remainder in terms of derivatives to place upper bounds on $\sigma(r)$ for a few of the well-known integration formulae from equation (0.2.21). Since one expects that $\|f\|_{\Gamma_r}$ will increase with r while $\sigma(r)$ decreases the principle of minimising the product $\sigma(r).\|f\|_{\Gamma_r}$ with respect to r may be used.

Hammerlin also notes that if the quadrature rule is exact for polynomials of a fixed degree, n (say), and less then one can replace $\|f\|_{\Gamma_r}$ in equation (0.2.19) by $\|f-a\|_{\Gamma_r}$ where a is an arbitrary polynomial of degree n .

0.3 The Classical Approach

In contrast to Davis, Goodwin [14] used a more classical approach when obtaining expressions for the remainder in the evaluation of integrals of the form $\int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx$ by a repeated trapezoidal rule.

Let $\mathcal{R}$ be the rectangular contour $(\pm\infty \pm ih)$ and suppose that $f(z)$ is analytic on and within $\mathcal{R}$. Then from the theory of residues we have

$$(0.3.1) \qquad \int_{\mathcal{R}} \frac{f(z)\,e^{-z^2}}{1-e^{-2\pi i z/h}}\,dz = h\sum_{n=-\infty}^{\infty} e^{-n^2h^2} f(nh) .$$

Supposing $f(x)$ to be an even function we readily find that equation (0.3.1) becomes

$$(0.3.2)\quad \begin{cases} R(f) = \displaystyle\int_{-\infty}^{\infty} f(x)e^{-x^2}dx - h\sum_{n=-\infty}^{\infty} e^{-n^2h^2} f(nh) \\[2ex] \quad\;\; = -2\displaystyle\int_{-\infty-i\pi/h}^{\infty-i\pi/h} \frac{f(x)\,e^{-x^2}}{e^{2\pi i x/h}-1}\,dx \end{cases}.$$

Replacing x by $y - i\pi/h$ and noting that $\exp(-2\pi^2/h^2)$ is negligible compared to unity equation (0.3.2) becomes

$$(0.3.3)\qquad R(f) \doteq -2\,e^{-\pi^2/h^2}\int_{-\infty}^{\infty} f(y - i\pi/h)\,e^{-y^2}\,dy .$$

Assuming that the major contribution to the integral on the right of equation (0.3.3) is in the neighbourhood of $y = 0$ we find that the remainder term is given approximately by

$$(0.3.4)\qquad R(f) \doteq -2\,e^{-\pi^2/h^2} f(i\pi/h) .$$

This is, of course, Laplace's method for integrals, see De Bruijn [15, Chapt. IV] .

Equation (0.3.4) is a simple expression and usually gives good estimates. Goodwin notes that if $f(z)$ has a finite number of poles within $\mathcal{R}$ appropriate terms must be added from the calculation of the residues at these poles.

MacNamee [16] attempts to generalise Goodwin's result. MacNamee considers integrals over the semi-finite interval. The function $\pi g(z) \cot \pi(z/h - \lambda)$ is integrated round the rectangular contour $(0 \pm id, \mathcal{R} \pm id)$ and $\mathcal{R}$ is allowed to become infinite. Here λ is a parameter such that $0 \leq \lambda < 1$ and h is the tabular interval.

If $g(x)$ tends to zero as we let x become large and if there are no singularities of $g(z)$ within the rectangle we find that

$$(0.3.5) \qquad \int_0^\infty g(x)\,dx = h \sum_{n=0}^{\infty}{}' g\left[(n+\lambda)h\right] + E(\lambda,h,d) + C(\lambda,h,d)$$

where $\sum'$ denotes a sum whose first term is halved when $\lambda = 0$.

$E(\lambda, h, d)$ is called the error term and is the contribution from the integral along the sides of the rectangle parallel to the x-axis.

The emphasis of the paper is however placed on the correction term $C(\lambda, h, d)$ which is the contribution from the line through O parallel to the imaginary axis. The line is suitably indented at the origin when $\lambda = 0$.

MacNamee evaluates $C(\lambda, h, d)$ by the trapezoidal rule. Using the same method as above but with a rectangular contour of finite dimensions he obtains further correction and error terms. The method is again repeated and under certain conditions the integral on the right of equation (0.3.5) will be given by a series of trapezoidal sums with the remainder given approximately by the next correction term.

A process for controlling the error term $E(\lambda, h, d)$ by suitably choosing the parameters h and d is also outlined.

The second part of the paper is devoted to a discussion of the remainder in Gaussian integration rules. The remainder term is given by the contour integral

(0.3.6) $$R_{n+1}(f) = \frac{1}{2\pi i}\int_C \frac{q_{n+1}(z)}{p_{n+1}(z)} f(z)\, dz$$

where

(0.3.7) $$p_{n+1}(z) = (z - x_{0,n})(z - x_{1,n}) \ldots (z - x_{n,n})$$

and

(0.3.8) $$q_{n+1}(z) = \int_a^b \frac{\omega(x)\, p_{n+1}(x)}{z - x}\, dx .$$

C is any contour surrounding the basic interval $[a, b]$ and is such that $f(z)$ is regular on and within C. Equation (0.3.6) is readily obtained from an integration of the well-known expression for the remainder in interpolation formulae in terms of a contour integral, see e.g. Szegö [17] .

Bounds for $R_{n+1}(f)$ given by equation (0.3.6) are obtained by using the first term in the asymptotic expansion of $q_{n+1}(z)/p_{n+1}(z)$

for large $|z|$. MacNamee chooses the contour C to be a circle of radius $\mathcal{R}$. An upper bound is placed on $g(z)$ on C and the minimising technique used by Davis and Rabinowitz [9] and Hammerlin [13] is invoked.

MacNamee notes that it should not be difficult to allow a finite number of poles within C. The discussion is restricted to Gauss-Legendre, Gauss-Laguerre and Gauss-Hermite quadrature rules.

Stenger [18] also makes use of complex variable methods for placing bounds on the error in Gauss-type quadratures. He notes that the results of Davis and Rabinowitz [9] , Hammerlin [11] , [13] and MacNamee [16] can be made sharper by using the fact that the integration formulae are exact for polynomials of a known degree. For example in Davis' work the inequality (0.2.6) may be replaced by

$$(0.3.9)\qquad |R_{n+1}(f)|^2 \leq \sum_{k=0}^{\infty} |a_{2n+2k+1}|^2 \cdot \sum_{k=0}^{\infty} R_{n+1}\left[\zeta_k(z,\rho)\right]^2 ,$$

since the Gaussian formula using $n+1$ ordinates is correct for polynomials of degree less than or equal to $2n+1$.

Stenger then discusses the remainder term as used by MacNamee [16] in the form

$$(0.3.10)\qquad R_{n+1}(f) = \frac{1}{2\pi i}\int_C \left\{ \int_{-1}^{1} \frac{\omega(x)\, p_{n+1}(x)\, f(z)}{(z-x)\; p_{n+1}(z)} \cdot dx \right\} dz ,$$

where C is chosen to be the circle $|z| = 1+\varepsilon,\ \varepsilon > 0$. The function $f(z)$ is supposed analytic on and within C and has the Taylor series expansion within C given by

(0.3.11) $$f(z) = \sum_{k=0}^{\infty} a_k z^k .$$

Also, it is shown that

(0.3.12) $$\int_{-1}^{1} \frac{w(x)\, p_{n+1}(x)\, dx}{(z-x)\, p_{n+1}(z)} = \sum_{k=0}^{\infty} e_{n+1,k}\, z^{-2n-2k-3}$$

where the $e_{n+1,k} \geq 0$, $k = 0, 1, 2, \ldots$.

Substituting the infinite series given by equation (0.3.12) and equation (0.3.11) into equation (0.3.10) and integrating it is found that

(0.3.13) $$R_{n+1}(f) = \sum_{k=0}^{\infty} a_{2n+2k+2} \cdot e_{n+1,k} .$$

Using Schwarz's inequality, equation (0.3.13) gives

(0.3.14) $$|R_{n+1}(f)|^2 \leq \sum_{k=0}^{\infty} (e_{n+1,k})^2 \cdot \sum_{k=0}^{\infty} |a_{2n+2k+2}|^2 .$$

[Stenger in fact uses the more general Hölder inequality but the most useful result is given by equation (0.3.14).]

The quantity $\left\{ \sum_{k=0}^{\infty} (e_{n+1,k})^2 \right\}^{1/2}$ is given for a few of the well-known rules. The minimising technique of Davis and Rabinowitz [9] is again used.

All of the papers so far which have used complex variable techniques have made no attempt to deal with singularities in the range of integration. In the paper by Davis and Rabinowitz [9] the first assumption is that $f(z)$ is analytic on $[-1, 1]$ while Hammerlin [10] goes even further in assuming that $f(z)$ is analytic on and within the unit circle. Neither of these methods is of any use in dealing with singularities of $f(z)$ in the range of integration and their value when $f(z)$ has a singularity near the range of integration is doubtful.

On the other hand MacNamee [16] can deal with poles near the range of integration but his method again cannot be used when $f(z)$ has a singularity in the range of integration.

0.4 Barrett's Paper

Barrett [19] does discuss singularities of branch type at the end points of the integration interval. The emphasis of Barrett's paper is on the convergence properties of the Gaussian quadrature formulae and very little mention is made of estimates of the remainder term.

It is however around this paper that much of this thesis revolves and we will discuss the content in some detail.

Suppose $f(z)$ is analytic on and within a contour C which surrounds the basic interval $[a, b]$. Then from Cauchy's theorem we have

$$(0.4.1) \qquad f(x) = \frac{1}{2\pi i} \int_C \frac{f(z)}{z-x}\, dz .$$

Substituting this expression for $f(x)$ into equation (0.1.2) we find

$$(0.4.2) \qquad R_{n+1}(f) = \frac{1}{2\pi i} \int_C \frac{q_{n+1}(z)}{p_{n+1}(z)} f(z)\, dz$$

where

$$(0.4.3) \qquad p_{n+1}(z) = \prod_{k=0}^{n} (z - x_{k,n})$$

and

$$(0.4.4) \qquad q_{n+1}(z) = \int_a^b \frac{\omega(x)\, p_{n+1}(x)}{z-x}\, dx .$$

(Equation (0.4.2) is of course the expression for the remainder as used by MacNamee [16] , equation (0.3.6), but it should be pointed out that Barrett's paper was published before that of MacNamee.)

Barrett uses known asymptotic expressions for the ratio $q_{n+1}(z)/p_{n+1}(z)$ for large n in the case of Gauss-Jacobi integration formulae to obtain, for large n, expressions for the remainder in the two cases:

(1) when $f(z)$ is a meromorphic function;

(2) when $f(z)$ has a branch singularity at an end point of the range.

[The process contrasts with that of MacNamee in that MacNamee used asymptotic expressions for large values of $|z|$ while obtaining his estimates of $R_{n+1}(f)$.]

The contour in case (2) is chosen by Barrett to cross the interval $[-1, 1]$. This is however not permissible since, as we shall show later, $[-1, 1]$ is the cut in the complex plane for $q_{n+1}(z)$

Corresponding results are obtained for Gauss-Laguerre and Gauss-Hermite quadrature rules.

In the second part of the paper Barrett describes a process which generalises some of the ideas in Gaussian quadrature formulae. It is from this generalisation that the main theorem of this thesis stems.

Barrett chooses two functions of z, $\phi(z)$ which has simple zeros at each of the abscissae $x_{k,n}$, $k = 0(1)n$, and $\psi(z)$ which satisfies the condition

$$(0.4.5) \qquad \psi(x-0i) - \psi(x+0i) = 2\pi i\, w(x)\, \phi(x)$$

for $a < x < b$.

If we now put

$$(0.4.6) \qquad \lambda_{k,n} = -\frac{\psi(x_{k,n})}{\phi'(x_{k,n})}$$

into equation (0.1.2) it can be shown that the remainder in the quadrature rule is given by

$$(0.4.7) \qquad R_{n+1}(f) = \frac{1}{2\pi i}\int_C \frac{\psi(z)}{\phi(z)} f(z)\, dz$$

where C is a contour surrounding the basic interval $[a,b]$ and is such that $f(z)$ is regular on and within C.

Contours again appear to cross the cut for $\psi(z)$.

Barrett uses this result to find two new formulae, one corresponding to the Gauss-Laguerre formula which he terms the Gauss-Bessel integration formula, and the other corresponding to the Gauss-Hermite formula which is a repeated trapezoidal rule.

The contour integral obtained by Barrett is used only for dealing with meromorphic functions and functions with branch type singularities at the end points of the interval of integration.

As we have already stated Barrett's main interest is in the convergence properties of the various Gaussian Rules. No attempt is made to deal with entire functions.

In Chapter I of the thesis we shall state and prove our fundamental theorem which develops Barrett's treatment and puts it on a more rigorous basis. In this development we can deal with functions which not only have branch type singularities but also essential singularities at the end points of the interval of integration. The method used appears to overcome the difficulties involved at the end points. Our contour, unlike Barrett's, does not cross the cut in the complex plane.

Our aim is to find an expression for the remainder in many of the well-known formulae in terms of a contour integral. To achieve this we present a corollary of the main theorem. We shall use this corollary in the following chapter, Chapter II, to show how the main theorem yields an expression for the remainder in an important class of formulae which includes Gaussian and Newton-Cotes quadrature rules. We shall also give a second theorem which is a simple extension of the main theorem. This theorem leads to the corresponding contour integral expression for the remainder in osculatory quadrature formulae and formulae of Obreschkoff type, see e.g. Salzer [20] and [21] respectively.

In Chapter II we discuss the behaviour of the contour at the end points more fully. This behaviour depends on the function and the quadrature formula and we shall consider several of the more well-known rules.

The question of convergence of quadrature formulae is discussed in Chapter III. We follow the method of Barrett of examining the ratio $q_{n+1}(z)/p_{n+1}(z)$, for large n, in the contour integral expression for the remainder given by equation (0.4.2). We obtain Barrett's result for Newton-Cotes formulae using a slightly different procedure. [We note that Barrett's expression for $q_{n+1}(z)/p_{n+1}(z)$ is in error by a factor $1/n$]. The reason behind this is two-fold. Firstly, our method, unlike Barrett's, is immediately applicable to osculatory quadrature, and secondly, we find that our expression is more useful than Barrett's in a discussion of remainder estimates. We also discuss the convergence of Obreschkoff type formulae and Gaussian formulae.

In Chapter IV we use the contour integral expression for the remainder obtained in Chapter I to find asymptotic estimates of $R_{n+1}(f)$. Cases which will be discussed are

(1) functions with poles;

(2) functions with branch point singularities at the end points of the range;

(3) entire functions;

(4) functions with an essential singularity at an end point of the range.

In dealing with entire functions we shall make use of two methods. In the first we use the minimising technique of Davis and Rabinowitz [9] and Hammerlin [13] with respect to certain families of contours. The families of contours depend on the integration formulae. In the second we deform the contour to pass through the saddle points of the integrand and use the method of steepest descents, see e.g. De Bruijn [15, Chapt. ΣV] .

The second method is the one which would be used when finding estimates of the remainder when $f(z)$ has an essential singularity at an end point of the range of integration.

All our estimates are obtained under the assumption of large values of a parameter and it would appear that our results have limited use. However it is often found that expressions which are obtained in this way are extremely useful even for small values of the parameter. Elliott [22] and Elliott and Szekeres [23] obtain estimates for the coefficients a_n, $n = 0, 1, 2, \ldots$, in the Chebyshev series expansion of a function under the assumption of large values of n . The estimates yield surprisingly accurate results even for small values of . This idea is again used by Elliott [24] in a paper on the truncation errors in Padé approximations to functions. Luke [25] also mentions this unusual type of result in the introduction to a paper dealing with rational approximations to the incomplete Gamma-function.

In the conclusion we shall discuss a few of the problems that have presented themselves in the writing of this thesis. Firstly we have been unable to obtain a satisfactory expression for the ratio $\psi(z)/\varphi(z)$ occurring in equation (0.4.7) for Romberg's integration formula. Two possible ways in which we may be able to solve this problem are discussed. Secondly we shall consider how the fundamental theorem may be used to find new quadrature rules. We discuss one such formula which we term the 'Gauss-Whittaker' integration formula. Finally the original theme of this thesis, "a unification of quadrature formula", will be discussed. We shall consider how many of the known quadrature rules stem from the main theorem of Chapter I and consider a generalisation to the numerical integration of functions along a smooth arc in the complex plane. Barnhill [26] while discussing the convergence of complex integration formulae uses an expression for the remainder in terms of a contour integral which supposes that $f(z)$ is analytic on a contour which has the smooth arc in its interior. Our development allows singularities at the end points of the arc.

CHAPTER I

THE FUNDAMENTAL THEOREM

In this chapter we shall state and prove a result from which we may obtain an expression, in terms of a contour integral, for the remainder term of a general quadrature formula of the form given by equation (0.1.2). We recall that the formula may be written

$$\int_a^b \omega(x)\, f(x)\, dx = \sum_{k=0}^{n} \lambda_{k,n}\, f(x_{k,n}) + R_{n+1}(f). \tag{1.1.1}$$

The result as we have stated in section (0.4) has been previously outlined by Barrett [19]. Barrett however confines himself mainly to Gaussian quadrature formulae and to the integration of functions which are analytic in the basic interval $[a, b]$. Barrett also indicates possible changes when the function has either algebraic or logarithmic singularities at either or both of the end points a and b.

We shall generalise Barrett's results in our "fundamental theorem". The generalisation enables us to consider many more types of quadrature rules. Moreover we shall choose our contours with a twofold purpose in mind. Firstly, we shall be able to treat a wider class of functions than Barrett. We shall in fact be able to consider a function which has an essential singularity at the end point of the range. Secondly, our contours do not commit the error of crossing the cut in the complex plane.

We shall, then, choose our contours in such a way that we can prove the fundamental theorem for as wide a class of functions as we possibly can and so that we can apply the theorem to as many quadrature rules as we possibly can. However in the application of the theorem to specific functions and rules, we shall be able to deform the contours into one from which estimates are more easily obtained. A fuller discussion of the choice of contours is left to later chapters.

In stating the theorem we shall, in the first instance, confine ourselves to quadrature formulae in which the abscissae are all interior points of the interval of integration. A slight modification permits us later to deal with quadrature rules which have one or both of the end points as an abscissa/abscissae.

We also present a corollary of the fundamental theorem which gives an alternative definition of the function $\psi(z)$ occurring in the contour integral expression for the remainder. It is this form of $\psi(z)$ which we find most convenient for showing, in Chapter II, how the theorem may be used to obtain the remainder term, in the required form of a contour integral, for many of the well-known quadrature formulae.

A second theorem which is a generalisation of the fundamental theorem is then given. From this theorem we shall obtain the corresponding contour integral form for the remainder term in osculatory quadrature rules, see equation (0.1.3). This theorem as we shall point out has an extremely useful corollary similar to that of the fundamental theorem.

1.2 The Fundamental Theorem and A Corollary

Using the following theorem we shall be able to express the remainder $R_{n+}(f)$ in equation (1.1.1) with prescribed conditions on the weight factors $\lambda_{k,n}$, $k = 0(1)n$, in terms of a contour integral. We shall allow $f(z)$, the analytic continuation of $f(x)$ into the plane of the complex variable $z = x + iy$ to have a singularity at the end points of the interval $[a, b]$ but not at any point of the open interval (a, b).

In the first instance we shall consider only those quadrature formulae whose abscissae are interior points of $[a, b]$.

The fundamental theorem may be expressed as follows:

Theorem 1.

(i) Let $f(z)$ be a function of the complex variable, $z = x + iy$, analytic in some region D_1 of the complex plane which includes the open interval (a, b) in its interior.

(ii) Let $\phi(z)$ be an analytic function of z in the finite complex plane with simple zeros at each of the points $x_{k,n}$, $a < x_{k,n} < b$, $k = 0(1)n$. Suppose that all other zeros of $\phi(z)$ lie outside a region D_2 which has the closed interval $[a, b]$ in its interior.

(iii) $\psi(z)$ is an analytic function of z in the complex plane cut along the entire real axis.

(iv) $\psi(x - oi) - \psi(x + oi) = 2\pi i\, w(x)\, \phi(x)$ for all x lying in the open interval (a, b). We notice that for each k, $k = 0(1)n$, $\psi(x_{k,n})$ is uniquely defined since $\phi(x_{k,n})$ is zero.

(v) Define the quantity $R_{n+1}(f)$ by

$$(1.2.1) \qquad R_{n+1}(f) = \int_a^b w(x) f(x)\, dx - \sum_{k=0}^{n} \frac{\psi(x_{k,n})}{\phi'(x_{k,n})} \cdot f(x_{k,n}).$$

Then

$$(1.2.2) \qquad R_{n+1}(f) = \frac{1}{2\pi i} \left\{ \int_{C^+} + \int_{C^-} \right\} \frac{\psi(z)}{\phi(z)} f(z)\, dz \,,$$

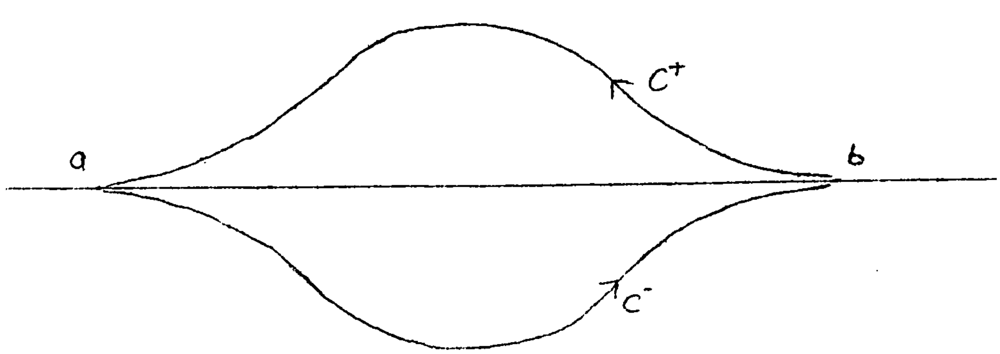
where the contours C^+ and C^-, see Figure 1.1, are open* contours between the points a and b satisfying the following conditions:

(1) C^+ and C^- are described in the positive (anti-clockwise), direction.

(2) C^+ and C^- are confined to the upper and lower half planes respectively in the region common to both D_1 and D_2.

(3) The slopes of C^+ at a and b are parallel to the negative direction of the x-axis while the slopes of C^- at a and b are parallel to the positive direction of the x-axis.

FIGURE 1.1



*An open contour is one which does not include its end points.

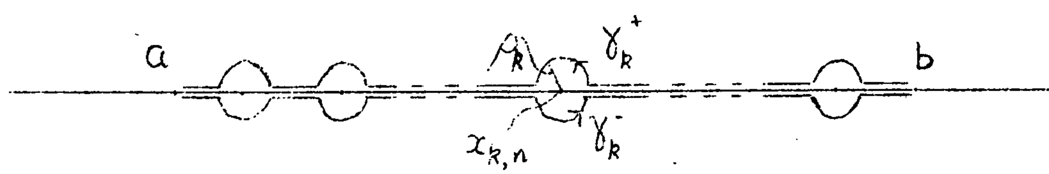
[<u>Note</u>: We choose the contours C^+ and C^- to be open contours because the function $\psi(z)f(z)/\phi(z)$ has in general a singularity at an end point due either to a singularity of $f(z)$ or possibly, as we shall show in Chapter II, to a singularity of $\psi(z)$.]

<u>Proof</u>: Since $\psi(z)f(z)/\phi(z)$ has no singularities between C^+ and the upper edge of the open interval (a, b) we may deform C^+ to be the upper edge of the open interval together with small semi-circles, γ_k^+ , at each of the points $x_{k,n}$, $k = 0(1)n$.

Let the radius of γ_k^+ be ρ_k .

Similarly we may deform C^- to be the lower edge of (a, b) with semi-circular indentations γ_k^- of radius ρ_k at the points $x_{k,n}$, $k = 0(1)n$, see Figure 1.2.

<u>FIGURE 1.2</u>



Under these circumstances the conditions on the slopes at the end points of both C^+ and C^- are conserved.

Let us denote by $R_{n+1}(f, \gamma_k^+)$ the contribution to $R_{n+1}(f)$ from the integral around the semi-circle γ_k^+. We have

$$(1.2.3) \qquad R_{n+1}(f, \gamma_k^+) = \frac{1}{2\pi i} \int_{\gamma_k^+} \frac{\psi(z)}{\varphi(z)} f(z)\, dz \quad .$$

Now the function $\psi(z) f(z)/\varphi(z)$ is analytic and therefore continuous on the semi-circle γ_k^+ Also the function $\varphi(z)$ has a simple zero at the point $z = x_{k,n}$

Therefore we have

$$(1.2.4) \qquad \lim_{z \to x_{k,n}} \left\{ (z - x_{k,n}) \frac{\psi(x_{k,n}) f(x_{k,n})}{\varphi(x_{k,n})} \right\} = \frac{\psi(x_{k,n}) f(x_{k,n})}{\varphi'(x_{k,n})}$$

provided we confine the path of the limit to the upper half-plane.

Letting the radius of the semi-circle γ_k^+ tend to zero we find that equation (1.2.3) yields, see Volkovyskii et al [27, p.67],

$$(1.2.5) \qquad R_{n+1}(f, \gamma_k^+) = \frac{1}{2} \cdot \frac{\psi(x_{k,n})}{\varphi'(x_{k,n})} \cdot f(x_{k,n}) \quad .$$

Similarly, since $\psi(x_{k,n})$ is uniquely defined,

$$(1.2.6) \qquad R_{n+1}(f, \gamma_k^-) = \frac{1}{2} \cdot \frac{\psi(x_{k,n})}{\varphi'(x_{k,n})} \cdot f(x_{k,n}) \quad .$$

Proceeding in this way for each k, $k = 0(1)n$ we have from equations (1.2.2), (1.2.5) and (1.2.6)

$$R_{n+1}(f) = \frac{1}{2\pi i}\int_b^a \frac{\psi(x+oi)}{\phi x} f(x)\,dx + \sum_{k=0}^{n}\frac{1}{2}\frac{\psi(x_{k,n})}{\phi'(x_{k,n})} f(x_{k,n}) + \tag{1.2.7}$$
$$+ \frac{1}{2\pi i}\int_a^b \frac{\psi(x-oi)}{\phi(x)} f(x)\,dx + \sum_{k=0}^{n}\frac{1}{2}\frac{\psi(x_{k,n})}{\phi'(x_{k,n})} f(x_{k,n}).$$

Using condition (4) of the Theorem equation (1.2.7) gives us

$$R_{n+1}(f) = \int_a^b \omega(x) f(x)\,dx + \sum_{k=0}^{n}\frac{\psi(x_{k,n})}{\phi'(x_{k,n})} f(x_{k,n}). \tag{1.2.8}$$

Application of the Theorem to Quadrature Formulae

In the quadrature formula (1.1.1) suppose that the abscissae are interior points of the interval $[a, b]$. Let us now assign to the weight factor, $\lambda_{k,n}$, in equation (1.1.1) the value given by

$$\lambda_{k,n} = -\frac{\psi(x_{k,n})}{\phi'(x_{k,n})}, \quad k = 0(1)\,n. \tag{1.2.9}$$

Then the remainder term, $R_{n+1}(f)$, is given in the required form by equation (1.2.2) of the fundamental theorem.

Comments on the Theorem

(1) We have chosen the function $\psi(z)$ to be analytic in the plane cut along the entire real axis because we may define $\psi(z)$ differently in the upper and lower half-planes. In many cases however the function $\psi(z)$ will be analytic in the complex plane cut along some finite part of the real axis. For example in the Gauss-Legendre quadrature rule $\psi(z)$ is analytic in the complex plane cut along $[-1, 1]$.

(2) In the application of the theorem to quadrature formulae it appears that the choice of the weight factors using equation (1.2.9) is very restricted. However we note that we may add to $\psi(z)$ an arbitrary function $P(z)$ which is analytic in the finite part of the complex plane without altering the conditions of the theorem.
We would replace $\psi(z)$ by $\psi(z) + P(z)$ throughout the theorem. This broadens considerably the scope of quadrature formulae. We shall return to this point later.

When the End Point is an Abscissa of the Quadrature Formula

So far we have confined ourselves to integration formulae in which the abscissae are interior points of the interval $[a, b]$. A slight modification gives the corresponding result when we have either or both of a and b as an abscissa/abscissae. We simply include the contribution(s) from the end point(s) in the remainder term.

Suppose that $a = x_{0,n}$ but that b is not an abscissa. Then we rewrite equation (1.1.1) in the form

$$\int_a^b w(x) f(x)\, dx = \sum_{k=1}^{n} \lambda_{k,n} f(x_{k,n}) + R_{n+1}^{x}(f) \tag{1.2.10}$$

where

$$R_{n+1}^{x}(f) = \lambda_{0,n} f(x_{0,n}) + R_{n+1}(f). \tag{1.2.11}$$

When the weight factors $\lambda_{k,n}$, $k = 1(1)n$, in equation (1.2.10) are given by an equation of the form (1.2.9) the theorem gives us an expression for $R_{n+1}^{x}(f)$ in terms of a contour integral. The only alteration to the proof is that we would not consider an indentation at the point $x_{0,n}$.

We would treat the case when b is an abscissa similarly. The fundamental theorem gives as a contour integral the remainder term of a quadrature formula where the weight factors, $\lambda_{k,n}$, $k = 0(1)n$, are given in terms of the functions $\psi(z)$ and $\phi(z)$ defined in the theorem. By choosing different functions $\psi(z)$ and $\phi(z)$ subject to the conditions of the theorem we obtain many quadrature rules.

The following corollary of the fundamental theorem gives under certain conditions an alternative definition for the function $\psi(z)$. We find this form of $\psi(z)$ extremely useful when considering particular quadrature rules.

Corollary 1: Let $\phi(z)$ and $\psi(z)$ be two functions of z satisfying the conditions of the fundamental theorem. Suppose now that $\phi(z)$ and $\psi(z)$ are subject to the following conditions:

(1) condition (iv) of the theorem holds not only for the interval (a, b) but also for an interval (c, d) which contains (a, b) and

$$\psi(x - oi) = \psi(x + oi) \tag{1.2.12}$$

for values of x not in the closed interval $[c, d]$. (The intervals (a, b) and (c, d) are in fact identical in many cases.)

(2) $\psi(z)$ tends to zero as $|z|$ tends to infinity.

(3) $\omega(x)\,\phi(x)$ satisfies a Hölder condition for x in the open interval (c, d). That is, we have

for any two points x_1 and x_2 of (c, d)

$$|\omega(x_1)\phi(x_1) - \omega(x_2)\phi(x_2)| \leqslant A \cdot |x_1 - x_2|^{\mu} \tag{1.2.13}$$

where A is a positive constant and $0 \leq \mu \leqslant 1$.

Then

$$\psi(z) = \int_c^d \frac{\omega(x)\,\phi(x)\,dx}{z - x} . \tag{1.2.14}$$

Proof: The proof follows immediately from a result given by Muskhelishvili [28, p.65].

Comments on the Corollary

(1) Suppose that we do not impose any condition on the behaviour of the function $\psi(z)$ as $|z|$ tends to infinity. Then we may choose, for $\psi(z)$,

$$\psi(z) = \int_a^b \frac{\omega(x)\,\phi(x)\,dx}{z - x} + P(z) \tag{1.2.15}$$

where $P(z)$ is an arbitrary function of z analytic in the finite complex plane, see Muskhelishvili [28, p.65]. By imposing condition (2) of the corollary we imply $P(z) = 0$.

(2) When the interval (c, d) is infinite we must impose the further conditions that the integral on the right hand side of

equation (1.2.14) exists.

The case of an infinite interval has also been discussed by Muskhelishvili [28, p.110] . Muskhelishvili states that a necessary, but certainly not sufficient condition for the existence of the integral, is given by

$$(1.2.16) \quad |\omega(x)\phi(x) - \omega(\infty)\phi(\infty)| < \frac{A_1}{|x|^\alpha}, \quad \alpha > 0,$$

for large values of x . A_1 is constant.

(3) For our purposes the Hölder condition, the inequality (1.2.13) will usually be too general. In most cases we shall require that $\omega(x)\phi(x)$ has a continuous first derivative in (c, d) This corresponds to $\mu = 1$ in equation (1.2.13) together with a condition which ensures the existence of $\psi(z)$ when the interval (c, d) is infinite.

1.3 Osculatory Quadrature Formulae

The corresponding expression in terms of a contour integral for the remainder term in osculatory quadrature formulae is readily obtained by means of a simple generalisation of the fundamental theorem. We recall that the osculatory quadrature formula may be written, see equation (0.1.3),

$$\int_a^b \omega(x)\, f(x)\, dx = \sum_{r=0}^{p-1} \sum_{k=0}^{n} \lambda_{k,r,n}\, f^{(r)}(x_{k,n}) + R_{(n+1)p}(f). \tag{1.3.1}$$

The following theorem enables us to express the remainder term $R_{(n+1)p}(f)$ in equation (1.3.1) with prescribed conditions on the weight factors $\lambda_{k,r,n}$, $k = 0(1)n$, $r = 0(1)\{p-1\}$, when the abscissae $x_{k,n}$, $k = 0(1)n$ are interior points of the interval $[a, b]$. Osculatory quadrature formulae in which the end points a and/or b are abscissae will be considered immediately after.

Theorem 2: (i) Suppose that the functions $\psi(z)$, $\phi(z)$ and $f(z)$ are three functions of z satisfying the conditions of the fundamental theorem except that $\phi(z)$ has not simple zeros but zeros of order p at each of the points $x_{k,n}$ where $a < x_{k,n} < b$.

(ii) define the quantity $R_{(n+1)p}(f)$ by

$$R_{(n+1)p}(f) = \int_a^b \omega(x)\, f(x)\, dx + \\ + \sum_{k=0}^{n} \frac{1}{(p-1)!} \left\{ \frac{d^{p-1}}{dz^{p-1}} \left[(z - x_{k,n})^p \frac{\psi(z) f(z)}{\phi(z)} \right] \right\}_{z = x_{k,n}}. \tag{1.3.2}$$

Then

$$R_{(n+1)p}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} \frac{\psi(z)}{\phi(z)} f(z)\,dz \tag{1.3.3}$$

where C^+ and C^- are contours of the type considered in the fundamental theorem.

Proof: The proof follows the same lines as that of the fundamental theorem except in the evaluation of the contribution to $R_{(n+1)p}(f)$ from the semi-circular indentations, $\gamma_k^{\pm}$, above and below $x_{k,n}$ as we let the radius ρ_k of the semi-circles tend to zero.

First we note that from condition (4) of the fundamental theorem $\psi(x_{k,n})$ is again uniquely defined. Furthermore it immediately follows that the derivatives of $\psi(z)$ up to and including the $(p-1)st$ derivative evaluated at the point $z = x_{k,n}$, $k = 0(1)n$, are also uniquely defined. This may be shown as follows.

From condition (4) of Theorem 1 we have

$$\psi(x-0i) - \psi(x+0i) = 2\pi i\, \omega(x)\, \phi(x) . \tag{1.3.4}$$

On repeated differentiation equation (1.3.4) gives

$$(1.3.5)\quad \begin{cases} \psi'(x-0i) - \psi'(x+0i) = 2\pi i\left[\omega'(x)\,\varphi(x) + \omega(x)\,\varphi'(x)\right], \\ \quad - \qquad - \qquad = \qquad - \qquad - \\ \quad - \qquad - \qquad = \qquad - \qquad - \\ \psi^{(p-1)}(x-0i) - \psi^{(p-1)}(x+0i) = 2\pi i\left[\omega^{(p-1)}(x)\,\varphi(x) + \cdots + \omega(x)\,\varphi^{(p-1)}(x)\right]. \end{cases}$$

Now since $\varphi(z)$ has a zero of order p at each of the points $x_{k,n}$, $k = 0(1)n$, then $\varphi(z), \varphi'(z), \ldots, \varphi^{(p-1)}(z)$ are all zero at $z = x_{k,n}$, $k = 0(1)n$. Thus the equations (1.3.5) show us that $\psi(z), \psi'(z), \ldots, \psi^{(p-1)}(z)$ are uniquely defined at each of these points.

The right hand side of equation (1.3.2) contains $\psi(z)$ and only its first $(p-1)$ derivatives evaluated at $z = x_{k,n}$, $k = 0(1)n$. Therefore the fact that $\psi(z)$ and its first $(p-1)$ derivatives are uniquely defined at these points ensures that equation (1.3.2) is defined uniquely.

Now $\varphi(z)$ has a zero of order p at $z = x_{k,n}$. So that

$$(1.3.6)\qquad \varphi(z) = (z - x_{k,n})^p\, \varphi_1(z)$$

where $\varphi_1(z)$ is analytic at $z = x_{k,n}$.

Therefore for z on the semi-circle γ_k^+ we may write

$$(1.3.7)\qquad \frac{\psi(z)}{\varphi(z)} \cdot f(z) = \frac{\alpha_0}{(z-x_{k,n})^p} + \frac{\alpha_1}{(z-x_{k,n})^{p-1}} + \cdots + \frac{\alpha_{p-1}}{z-x_{k,n}} + A(z)$$

where, for $\nu = 0(1)\{p-1\}$,

$$(1.3.8) \qquad \alpha_\nu = \lim_{z \to x_{k,n}^+} \frac{1}{\nu!} \frac{d^\nu}{dz^\nu} \left[\frac{\psi(z) f(z)}{\varphi_1(z)} \right]$$

and $A(z)$ is a bounded function of z.

Similarly for z on the semi-circle γ_k^- we have

$$(1.3.9) \qquad \frac{\psi(z)}{\varphi(z)} \cdot f(z) = \frac{\beta_0}{(z-x_{k,n})^p} + \frac{\beta_1}{(z-x_{k,n})^{p-1}} + \cdots + \frac{\beta_{p-1}}{(z-x_{k,n})} + B(z)$$

where, for $\nu = 0(1)\{p-1\}$,

$$(1.3.10) \qquad \beta_\nu = \lim_{z \to x_{k,n}^-} \frac{1}{\nu!} \frac{d^\nu}{dz^\nu} \left[\frac{\psi(z)}{\varphi_1(z)} \cdot f(z) \right].$$

and $B(z)$ is another bounded function of z.

The coefficients α_ν and β_ν, $\nu = 0(1)\{p-1\}$ contain only uniquely defined quantities and hence

$$(1.3.11) \qquad \alpha_\nu = \beta_\nu \quad , \quad \nu = 0(1)\{p-1\}.$$

The bounded functions $A(z)$ and $B(z)$ are however different in general

Let us now evaluate the contributions $R_{(n+1)p}(f, \gamma_k^+)$ and $R_{(n+1)p}(f, \gamma_k^-)$ to the quantity $R_{(n+1)p}(f)$ from the integrals along the semi-circles γ_k^+ and γ_k^- respectively. We have from equations (1.3.7) and (1.3.9)

$$(1.3.12)\quad R_{(n+1)p}(f,\gamma_k^+) + R_{(n+1)p}(f,\gamma_k^-) = \frac{1}{2\pi i}\left\{\int_{\gamma_k^+} + \int_{\gamma_k^-}\right\}\left[\frac{\alpha_0}{(z-x_{k,n})^p} + \cdots + \frac{\alpha_{p-1}}{(z-x_{k,n})}\right]dz + \frac{1}{2\pi i}\int_{\gamma_k^+} A(z)\,dz + \frac{1}{2\pi i}\int_{\gamma_k^-} B(z)\,dz .$$

Since both $A(z)$ and $B(z)$ are bounded functions of z on γ_k^+ and γ_k^- respectively the last two integrals on the right of equation (1.3.12) tend to zero as we let the radii (ρ_k) and hence the lengths of the semi-circles tend to zero.

Further, substituting $(z - x_{k,n}) = \rho_k e^{i\phi}$ in the first integral we find that

$$(1.3.13)\quad \frac{1}{2\pi i}\left\{\int_{\gamma_k^+} + \int_{\gamma_k^-}\right\}\left[\frac{\alpha_0}{(z-x_{k,n})^p} + \cdots + \frac{\alpha_{p-1}}{(z-x_{k,n})}\right]dz = \alpha_{p-1} .$$

Therefore letting ρ_k tend to zero equation (1.3.12) gives us

$$(1.3.14)\quad R_{(n+1)p}(f,\gamma_k^+) + R_{(n+1)p}(f,\gamma_k^-) = \alpha_{p-1} .$$

Now α_{p-1} is the residue of $\psi(z)f(z)/\phi(z)$ evaluated at $z = x_{k,n}$. Therefore, see Fuchs and Shabat [29, p.265],

$$(1.3.15)\quad \alpha_{p-1} = \lim_{z\to x_{k,n}} \frac{1}{(p-1)!}\frac{d^{p-1}}{dz^{p-1}}\left[(z-x_{k,n})^p\frac{\psi(z)}{\phi(z)}f(z)\right] .$$

The proof is completed by following the steps of the fundamental theorem.

Application of Theorem 2 to Osculatory Quadrature Formulae

Suppose that the abscissae in the quadrature formula given by equation (1.3.1) are interior points of the interval. Now let us assign to the coefficients $\lambda_{k,r,n}$ the value given by

$$(1.3.16) \qquad \lambda_{k,r,n} = \frac{-\binom{p-1}{r}}{(p-1)!}\left\{ \frac{d^{p-1-r}}{dz^{p-1-r}}\left[(z-x_{k,n})^{p}\frac{\psi(z)}{\varphi(z)}\right]\right\}_{z=x_{k,n}}$$

for $k = 0(1)n$, $r = 0(1)\{p-1\}$.

We see that $\lambda_{k,r,n}$ is the coefficient of $f^{(r)}(x_{k,n})$ in the expression for α_{p-1} given by equation (1.3.15).

Thus, from Theorem 2, the remainder term in osculatory quadrature formulae when the coefficients are defined by equation (1.3.16) is given by

$$(1.3.17) \qquad R_{(n+1)p}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\}\frac{\psi(z)}{\varphi(z)}\cdot f(z)\,dz$$

where C^{+} and C^{-} are contours of the type considered in the fundamental theorem, see Fig. 2.1.

When an End Point is an Abscissa

As in the case of the fundamental theorem a slight modification gives the corresponding result when an end point is an abscissa. We simply modify the formula to include the contribution from the end point in the remainder term. Suppose that $a = x_{0,n}$ but that b is not an abscissa. Then Theorem 2 gives an expression in terms of a contour integral for $R^{X}_{(n+1)p}(f)$ in the formula

$$\int_a^b \omega(x) f(x)\,dx = \sum_{k=1}^{n} \sum_{r=0}^{p-1} \lambda_{k,r,n} f^{(r)}(x_{k,n}) + R^{X}_{(n+1)p}(f) \tag{1.3.18}$$

where

$$R^{X}_{(n+1)p}(f) = R_{(n+1)p}(f) + \sum_{r=0}^{p-1} \lambda_{0,r,n} f^{(r)}(x_{0,n}) . \tag{1.3.19}$$

A Corollary of Theorem 2

The function $\psi(z)$ in osculatory quadrature rules may be defined alternatively using a corollary similar to the corollary of the main theorem. The corollary may be stated as follows.

Corollary 2: (1) Let $\phi(z)$ and $\psi(z)$ satisfy the conditions of Theorem 2.

(2) Suppose that $\varphi(z)$ and $\psi(z)$ satisfy the conditions of corollary 1.

Then we have similarly

$$\psi(z) = \int_c^d \frac{\omega(x)\,\varphi(x)}{z-x}\,dx \qquad (1.3.20)$$

Comments on Theorem 2 and its Corollary

(1) We note that as in the fundamental theorem we may add an analytic function $P(z)$ to $\psi(z)$ without altering the theorem. Again we see that this broadens our choice of the coefficients considerably.

(2) When the interval (c, d) in equation (1.3.20) is infinite we must impose the condition that the integral on the right of the equation exists.

Corollary 2 will be used to obtain an expression for the remainder term in the integration formula derived from the Hermite interpolation formula which uses only the value of the function and its derivatives at each of the abscissae

We also find this corollary extremely useful when considering formulae of Obreschkoff type, see Salzer [21] , which use the value of the function and its derivatives up to any order at only the end points of the range.

The integration formula given by equation (1.3.1) could be further generalised to formulae which involve derivatives of varying orders at each of the abscissae, for example, the integration of the general Hermite interpolation formula, see Spitzbart [30] . Although our method is readily adapted to such formulae we shall not consider them any further in this thesis.

CHAPTER II

THE APPLICATION OF THE FUNDAMENTAL THEOREM TO SPECIFIC QUADRATURE FORMULAE

2.1 Introduction

In Chapter I an expression for the remainder term in a general quadrature formula of the form of equation (0.1.2) or equation (0.1.3) was obtained in terms of a contour integral. The contours were chosen in such a way as to avoid singularities of the function $[\psi(z) f(z)/\phi(z)]$ at either end point of the interval $[a, b]$.

In the first part of this chapter we shall discuss the possible singularities at the end point a. A similar discussion holds for the end point b.

Now all three functions $\psi(z)$, $\phi(z)$ and $f(z)$ may be sources of a singularity at a.

Firstly $\psi(z)$ does not in general tend to a finite limit as z approaches a. We shall discuss the behaviour of $\psi(z)$ near a more fully in Section 2 of this chapter.

Secondly the end point a may be an abscissa of the quadrature rule as in the Newton-Cotes formula. In this case we see from condition (2) of the theorem that the function $\phi(z)$ has a zero at a and hence $[\psi(z)\, f(z)/\phi(z)]$ has a pole at that end point.

Finally we recall that the function $f(z)$ was supposed to be analytic in a region D_1 of the complex plane which included in its interior the real interval $[a, b]$ with perhaps the exception of the end points a and b. This was done in order that we may allow $f(z)$ to have a singularity at a.

Once the type of singularity at the end point a is known we need not confine the behaviour of the contour to that specified in the fundamental theorem. In Section 3 of this chapter we shall discuss the alternative behaviours of the contours C^+ and C^- at the end point a when the function $f(z)$ falls into one of the following categories:

(a) $f(z)$ has no singularities on $[a, b]$;

(b) $f(z)$ has a branch singularity at the end point a;

(c) $f(z)$ has an essential singularity at a.

We shall take into account the case when the end point is an abscissa and show how we may obtain a contribution to the quadrature sum from the end point.

In Section 4 we shall show how the fundamental theorem and its corollary may be used to give an expression for the remainder term in many well-known numerical integration formulae. We shall discuss the behaviour of the contours at the end points in the formulae of Newton-Cotes and formulae of Gaussian type.

A useful illustration of how the contour may be chosen at the end point is provided by the repeated trapezoidal rule. From this discussion of the repeated trapezoidal rule we shall obtain the results used by MacNamee [16] and Goodwin [14] together with the classical Abel-Plana form of the remainder, see e.g. Whittaker and Watson [31, p.145] .

In Section 2.4(e) we shall discuss osculatory quadrature formulae and formulae of Obreschkoff type.

In an extremely important case the contours C^+ and C^- combine to give a single closed contour. We shall, in Section 2.5, conclude this chapter by discussing conditions under which such a contour can be chosen.

2.2 The Behaviour of $\psi(z)$ near the End Point a

To enable us to discuss fully the choice of the contours C^+ and C^- at the end point a we need to know how the function $\psi(z)$ behaves near a.

In general, when all that is known about $\psi(z)$ is that it satisfies the conditions of the fundamental theorem we may not be able to say much about the behaviour of that function in a neighbourhood of a. When, of course, an explicit expression for $\psi(z)$ in terms of transcendental functions is known the behaviour of $\psi(z)$ is readily ascertained.

On the other hand for many quadrature formulae it is found that the functions $\psi(z)$ and $\varphi(z)$ satisfy the conditions of Corollary 1. Under these circumstances the behaviour of $\psi(z)$ near the end point a has been firmly established.

We notice first that if the end point a is an abscissa of the quadrature formula $\varphi(a) = 0$. Hence $\psi(z)$ is uniquely defined at a as it is at all the abscissae of the quadrature rule.

Let us then consider the case when a is not an abscissa of the quadrature formula.

If the functions $\varphi(z)$ and $\psi(z)$ satisfy the conditions of Corollary 1 then we have

$$(2.2.1) \qquad \psi(z) = \int_c^d \frac{\omega(x)\,\phi(x)}{z - x}\,dx \quad .$$

Now $\phi(z)$ does not have a singularity at any point of the interval of integration $[a, b]$. However the weight function, as we have indicated in Section 0.1 of the Introduction, may have an algebraic or logarithmic singularity at either end point of the interval $[a, b]$.

Let us then write for z near a

$$(2.2.2) \qquad \omega(z) = (z-a)^{\sigma}\,\omega_0(z)$$

where $\omega_0(z)$ is an analytic function of z near a and $-1 < \sigma \leq 0$.

There are two separate cases to consider:

(i) when the end point c of the cut $[c, d]$ for the function $\psi(z)$ coincides with the end point a of the interval of integration $[a, b]$, i.e. when $c = a$;

(ii) when $c < a$ and hence the interval of integration $[a, b]$ is properly contained in $[c, d]$.

(i) When $c = a$.

When c coincides with a then $\omega(x)\varphi(x)$ need not necessarily be defined at the end point a in order that the Hölder condition (1.2.13) may be satisfied. Therefore the weight function may be of the form given by equation (2.2.2). Thus, from Muskhelishvili [28, para.29] the behaviour of $\psi(z)$ for z near a but not in $[a, b]$ is as follows:

(a) when $-1 < \sigma < 0$ we have

$$\psi(z) = \frac{e^{\sigma\pi i}(z-a)^{\sigma}\,\omega_0(a)\,\varphi(a)}{2i\sin\sigma\pi} + \psi_0(z) \tag{2.2.3}$$

with

$$|\psi_0(z)| < C\,|z-a|^{\sigma_0} \tag{2.2.4}$$

where $\sigma_0 > \sigma$ and C is a real constant;

(b) when $\sigma = 0$ we have

$$\psi(z) = \frac{\omega_0(a)\,\varphi(a)}{2\pi i}\cdot\log\left[\frac{1}{z-a}\right] + \psi_0(z) \tag{2.2.5}$$

where $\psi_0(z)$ is a bounded function of z near and at the end point a.

(ii) When $c < a$.

When $c < a$ the function $\omega(x)\varphi(x)$ satisfies the Hölder condition (1.2.13) at the point a. Hence the weight function must be clearly defined at that end point, that is σ in equation (2.2.2) must be greater than or equal to zero.

In this case, see Muskhelishvili [28, p.27], the function $\psi(z)$ is a continuous function of z as z approaches points of the open interval (c, d) and in particular as z approaches the point a. Furthermore as z tends to a, $\psi(z)$ tends to a definite limit which depends on whether the path of the limit is in the upper or lower half-planes.

Results similar to these hold for z near a and on the interval $[a, b]$.

The above results may be summed up as follows:

If the functions $\psi(z)$ and $\varphi(z)$ satisfy the conditions of Corollary 1 then in all possible cases the ratio $\psi(z)/\varphi(z)$ may be expressed in the form,

(2.2.6) $$\frac{\psi(z)}{\varphi(z)} = (z-a)^{\sigma} \cdot g(z)$$

where $-1 \leq \sigma \leq 0$ and $g(z)$ satisfies the following conditions:

(i) in the upper half-plane and in the lower half-plane $g(z)$ is a bounded continuous function of z in the neighbourhood of a ;

(ii) $$\lim_{z \to a} g(z) = \begin{cases} g_1(a) & \text{when the path of the limit lies in the sector } 0 < \arg(z-a) < \pi, \\ g_2(a) & \text{when the path of the limit lies in the sector } \pi < \arg(z-a) < 2\pi. \end{cases}$$

When $-1 \leq \sigma < 0$, $\psi(z)/\varphi(z)$ <u>has</u> a singularity at a. If this is the case $g_1(a) = g_2(a)$. This follows from equations (2.2.3) and (2.2.5) when $-1 < \sigma < 0$, $c = a$, and the fact that $\psi(z)$ is uniquely defined at a when a is a zero of $\varphi(z)$.

<u>Osculatory Quadrature Formulae</u>

The corresponding results for osculatory quadrature formulae may be obtained similarly.

When the end point a is an abscissa the function $\varphi(z)$ has a zero of order p (see Theorem 2) at a while $\psi(z)$ is uniquely defined.

When a is not an abscissa we may follow the arguments used above in the case of the non-osculatory quadrature rules to obtain the form of the function $\psi(z)$ near the point a.

Thus for osculatory quadrature formulae when the functions $\psi(z)$ and $\phi(z)$ satisfy the conditions of Corollary 2 the ratio $\psi(z)/\phi(z)$ behaves like $(z-a)^{\sigma} g(z)$ where $\sigma > -1$ or $\sigma = -1, -2, \ldots, -p$ and $g(z)$ is bounded near and at a .

Having thus established the nature of the singularity of the function $\psi(z)/\phi(z)$ at a , subject to the conditions of Corollaries 1 and 2 we are now in a position to investigate fully the behaviour of the contours C^+ and C^- at the end point a of the interval of integration.

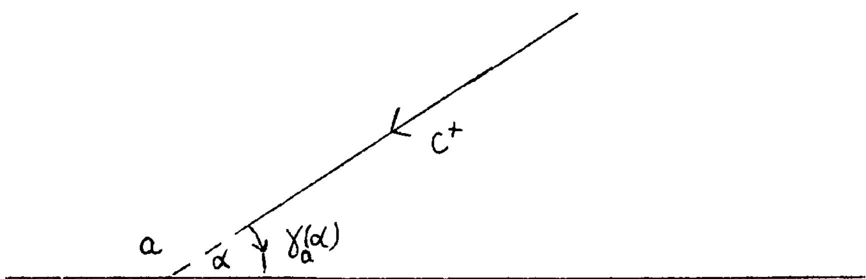
2.3 The Choice of the Contour C^+ at the End Point a

In the fundamental theorem of Chapter I the slope of the contour C^+ in the neighbourhood of the point was chosen to be parallel to the negative direction of the x-axis. This choice was made to avoid any discussion of a possible singularity at a of the function $\psi(z) f(z)/\phi(z)$.

For suppose that C^+ is chosen to approach a at an angle α, $0 < \alpha < \pi$, with the positive direction of the real axis. Since there may be a singularity at the end point a an indentation of the contour C^+ must be made as in the case of each of the abscissae of the quadrature formula. Suppose we take this indentation to be the arc $\gamma_a(\alpha)$ (angle α) of a circle with radius ρ and centre a described in the clockwise direction, see Fig. 2.1.

To establish the contour integral form of the remainder for the given quadrature formula we let the radius ρ of the arc $\gamma_a(\alpha)$ tend to zero. We must now be able to show that the integral of the function $\psi(z)\, f(z) \,/\, \phi(z)$ along $\gamma_a(\alpha)$ tends to a finite limit as ρ tends to zero. In the fundamental theorem α was taken to be zero and there was nothing to show.

FIGURE 2.1



In most cases we shall be able to relax the condition that the angle α is equal to zero. We may be able to show that as we let ρ tend to zero the integral along $\gamma_a(\alpha)$ tends to zero or contributes (usually when a is an abscissa) to the quadrature sum.

Consider first those formulae which do not involve derivatives of the function $f(x)$ in the quadrature sum, that is, non-osculatory quadrature formulae. To help in our discussion we shall require the following Lemma.

Lemma 1: Suppose that in the sector $0 < \arg(z-a) < \alpha$ the function $G(z)$ satisfies the conditions;

(i) $G(z)$ is continuous and bounded in the neighbourhood of the point a ;

(ii) $\lim_{z \to a} G(z) = G(a)$ for any path lying in sector $0 < \arg(z-a) < \alpha$.

Then if $\gamma_a(\alpha)$ is the arc, angle α, of a circle with radius ρ and centre a described in the clockwise direction

$$\lim_{\rho \to 0} \int_{\gamma_a(\alpha)} (z-a)^\sigma G(z)\, dz = \begin{cases} 0 & , \quad \sigma > -1 , \\ -i\alpha G(a) & , \quad \sigma = -1 . \end{cases}$$

Proof: Suppose $\sigma > -1$. Then it is readily shown that if $M(\rho)$ is an upper bound for $|G(z)|$ on $\gamma_a(\alpha)$

(2.3.1) $$\int_{\gamma_a(\alpha)} (z-a)^\sigma G(z)\, dz \leq M(\rho)\, \rho^{1+\sigma} \cdot \alpha .$$

The right hand side of the inequality (2.3.1) tends to zero with ρ since $\sigma > -1$.

On the other hand suppose $\sigma = -1$.

Then we may write for z near a and in the sector $0 < \arg(z-a) < \alpha$

$$G(z) = G(a) + G_0(z) \tag{2.3.2}$$

where

$$G(a) = \lim_{z \to a} G(z) \tag{2.3.3}$$

and

$$\lim_{z \to a} G_0(z) = 0 \tag{2.3.4}$$

Therefore

$$\int_{\gamma_a(\alpha)} (z-a)^{-1} G(z)\,dz = G(a)\int_{\gamma_a(\alpha)} \frac{dz}{z-a} + \int_{\gamma_a(\alpha)} \frac{G_0(z)\,dz}{z-a} . \tag{2.3.5}$$

On putting $(z-a) = \rho e^{i\varphi}$ in the first integral on the right of equation (2.3.5) we find

(2.3.6) $$G(a)\int_{\gamma_a(\alpha)} \frac{dz}{z-a} = -i\, G(a)\,\alpha .$$

Also if $M_0(\rho)$ is an upper bound for $|G_0(z)|$ on $\gamma_a(\alpha)$ then the second integral on the right of equation (2.3.5) is bounded above by

(2.3.7) $$M_0(\rho)\cdot\alpha .$$

Letting ρ tend to zero we see from equation (2.3.4) that $M_0(\rho)$ tends to zero. Hence equations (2.3.5) and (2.3.6) give us

(2.3.8) $$\lim_{\rho\to 0}\int_{\gamma_a(\alpha)} (z-a)^{-1} G(z)\,dz = -i\, G(a)\,\alpha .$$

This proves the Lemma.

<u>Note</u>: It is obvious that when the conditions of the Lemma are true for an angle α they are certainly true for any angle less than α (and of course greater than zero). Thus there is an element of choice in the slope of the contour at the end point. This choice is most important when there is a non-zero contribution from the integral along the arc. We shall find in this case that the angle α is usually determined by the requirements of the quadrature sum. This will be illustrated when we consider the repeated trapezoidal rule in Section 2. 4.

Formulae Satisfying the Conditions of Corollary 1

When the functions $\psi(z)$ and $\varphi(z)$ satisfy the conditions of Corollary 1 the type of singularity of the ratio $\psi(z)/\varphi(z)$ at the end point a is determined by Section 2.2. Any further singularity at a of the function $\psi(z) f(z)/\varphi(z)$ must be due to $f(z)$. Let us then examine the behaviour near a of the contour C^+ according to the singularity of $f(z)$ when the conditions of Corollary 1 are satisfied.

(a) When $f(z)$ has no singularity at a

Suppose $f(z)$ is analytic at the end point a. Then the singularity of $\psi(z) f(z)/\varphi(z)$ will be due to the singularity of the ratio $\psi(z)/\varphi(z)$.

Therefore for z near a and in the sector $0 < \arg(z-a) < \pi$ we may write

(2.3.9) $$\frac{\psi(z)}{\varphi(z)} \cdot f(z) = (z-a)^{\sigma} \cdot G(z)$$

where $\sigma \geqslant -1$ and the function $G(z)$ satisfies the conditions:

(1) $G(z)$ is bounded near a ,

(2) $\lim\limits_{z \to a} G_1(z) = G(a)$.

The conditions of Lemma 1 are, then, satisfied by the function $\psi(z) \cdot f(z) / \varphi(z)$ with $\alpha = \pi$.

Thus when $\sigma > -1$ the contribution for the integral along the arc tends to zero with ρ .

However, when the end point is an abscissa of the quadrature rule, $\sigma = -1$. Therefore from equations (2.3.8) and (2.3.9) the contribution from the integral along the arc $\gamma_a(\alpha)$ is $-i\, G(a) \cdot \alpha$.

Now

$$G_1(a) = \lim_{z \to a} (z-a) \cdot \frac{\psi(z) \cdot f(z)}{\varphi(z)} = \frac{\psi(a) \cdot f(a)}{\varphi'(a)} , \tag{2.3.10}$$

so that the contribution to the remainder term of the quadrature formula, equation (1.2.2), from the end point a is

$$- \frac{\alpha}{2\pi} \frac{\psi(a)}{\varphi'(a)} \cdot f(a) , \tag{2.3.11}$$

where we may take α to be any angle in the range $0 < \alpha < \pi$.

The term (2.3.11) is usually taken as part of the quadrature sum. The angle α will depend on the requirements of the quadrature rule; for example, as we shall show in Section 2.4(b), we choose $\alpha = \pi$ in the Newton-Cotes formula.

<u>(b) When $f(z)$ has a branch point at a</u>

When $f(z)$ has a branch point at a let us cut the plane from a along the real axis to $-\infty$.

It is found that there are two cases to consider:

(i) when $f(z)$ tends to a unique finite limit as z tends to a in the sector $0 < \arg(z-a) < \pi$;

(ii) when $f(z)$, for z near a, behaves like $(z-a)^\eta f_0(z)$ where $-1 < \eta < 0$ and $f_0(z)$ is analytic at a.

<u>Case (i)</u>: Combining the singularities of the ratio $\psi(z)/\phi(z)$ given in Section 2.2 with that of $f(z)$ we see that the function $\psi(z)f(z)/\phi(z)$ near a behaves like $(z-a)^\sigma G(z)$ where $\sigma \geqslant -1$ and $G(z)$ is bounded near a and tends to a unique limit as z tends to a in $0 < \arg(z-a) < \pi$.

The possible behaviour of C^+ at a is then similar to that in the case when $f(z)$ is analytic at a (Section 2.3(a)).

We may again take the angle α to be any angle less than or equal to π , and as we let the radius, ρ , of the arc tend to zero the integral will tend to zero or contribute to the quadrature sum.

Case (ii): Let us write

(2.3.12) $$f(z) = (z-a)^{\eta} f_0(z)$$

where $-1 < \eta < 0$ and $f_0(z)$ is analytic at a .

Now, so that the integral with which we are concerned exists, (the integral on the left of equation (0.1.1)) we must have

(2.3.13) $$\omega(z) = (z-a)^{\xi} \omega_0(z)$$

where $\eta + \xi > -1$ and $\omega_0(z)$ is analytic at a .

Also, since $f(z)$ is not defined at a a formula in which a is an abscissa would not be used. Therefore the only singularity of the ratio $\psi(z)/\phi(z)$ is that of the function $\psi(z)$. From equations (2.3.13) and (2.2.3) we see that for z near a

(2.3.14) $$\frac{\psi(z)}{\phi(z)} = (z-a)^{\xi} g(z)$$

where $g(z)$ is bounded near and at a.

From equations (2.3.12) and (2.3.14) we now have

$$\frac{\psi(z)}{\phi(z)} \cdot f(z) = (z-a)^{\sigma} \, G(z) \tag{2.3.15}$$

where $\sigma > -1$ and $G(z)$ satisfies the conditions of Lemma 1.

Thus the integral around the arc at a tends to zero as the radius, ρ, of the arc tends to zero.

<u>(c) When $f(z)$ has an essential singularity at a</u>

Suppose $f(z)$ has an essential singularity at the end point a then let us assume that there exists an angle $\beta \; (\geqslant 0)$ such that

$$\lim_{z \to a} f(z) = L \tag{2.3.16}$$

where the limit, L, is finite and independent of the path of the limit provided that this path is confined to the sector $0 \leq \arg(z-a) < \beta$. (Such an assumption ensures the existence of the real integral with which we are concerned, see equation (0.1.1)). As we have pointed out the angle may in fact be zero.

<u>Example</u>: As an example consider the function $e^{-1/z}$. We have

$$\lim_{z \to 0} e^{-1/z} = 0$$

provided the path of the limit is confined to the section $|\arg(z-a)| < \pi/2$. In the present discussion we would only be concerned with part of this sector, namely $0 < \arg(z-a) < \pi/2$.

From equation (2.2.6), which gives us the singularity at a of the ratio $\psi(z)/\phi(z)$, and equation (2.3.16), we see that the function $\psi(z)\,f(z)/\phi(z)$ behaves like $(z-a)^{\sigma}G(z)$ where $\sigma \geq -1$ and the function $G(z)$ is bounded near a and tends to a unique limit as z tends to a in the sector $0 \leq \arg(z-a) < \beta$.

We may take the angle, α, of the arc in this particular case to be any angle less than β. Using Lemma 1 we see that the contribution to the remainder term from the integral along the arc, $\gamma_a(\alpha)$, is zero for $\sigma > -1$ and equal to

$$-\frac{\alpha}{2\pi}\,\frac{\psi(a)}{\phi'(a)}\cdot L \tag{2.3.17}$$

for $\sigma = -1$.

<u>Note</u>: In cases (a) and (b) it was found that we could, in any particular situation, choose the angle of the arc to have any value less than π; the restriction of the angle is dependent somewhat on the cut for the function $\psi(z)$. In case (c), however, it is more likely that the angle of the arc will be governed by the nature of the essential singularity of the function $f(z)$.

The Behaviour of C^+ and C^- at the End Points a and b

Following the methods outlined above for the arc $\gamma_a(\alpha)$ above the end point a, the possible behaviours of C^- at a, and, C^+ and C^- at b alternative to those specified in the fundamental theorem may readily be obtained.

The above discussion gives us, then a choice within a specified range of the slopes of the contours C^+ and C^- at the end points a and b.

2.3(a) Osculatory Quadrature Formulae Satisfying Corollary 2

The discussion on the behaviour of the contours at the end points of the interval of integration when the quadrature formula satisfies the conditions of Corollary 1 is readily modified to deal with osculatory quadrature formulae which satisfy the conditions of Corollary 2.

When the end point is not an abscissa the arguments are exactly the same.

However when the end point is an abscissa we must be more restrictive. We recall that in the proof of Theorem 2, when considering the contributions from the indentations at an abscissa we took semi-circular arcs above and below the abscissa and dealt with them simultaneously. We must do likewise here.

Thus if we allow the slope of the contours at the end point to be any other than that specified in Theorem 2 we must take the angle of the arc above the end point a to be equal to π together with a similar arc below a. The contributions from these arcs are then considered simultaneously.

If we now follow that part of the proof of Theorem 2 concerning the contribution from the abscissae of the quadrature formula we find that the contribution from semi-circular arcs above and below a is given by (see equation (1.3.15))

$$(2.3.18) \qquad -\frac{1}{p!} \frac{d^{p-1}}{dz^{p-1}}\left[(z-a)^p \frac{\psi(z)}{\phi(z)} . f(z)\right]$$

evaluated at $z = a$.

We cannot take arcs which would not make a complete circuit of the end point a since the contribution from such an arc in the limit as the radius ρ of the arc tended to zero would not in general be finite.

We note at this point that if we use an osculatory quadrature formula in which the end point of the range is an abscissa both the function and its derivatives up to and including those of order p

must be uniquely defined there. This implies that we would not apply an osculatory quadrature formula with an abscissa at an end point of the interval of integration to a function which has an essential singularity at that end point.

Summing Up

Suppose the conditions of Corollary 1 are satisfied by the integration rule, then we may take the angles of the arcs above and below the end points to be any angles less than π (or perhaps some angle β (say) determined by an essential singularity at the end point) and we have

(i) when the end point is not an abscissa the contribution to the remainder from the integral around the arc tends to zero with the radius of the arc;

(ii) when the end point is an abscissa the contribution from an arc angle α is given by

(2.3.19) $$-\frac{\alpha}{2\pi}\,\frac{\psi(a)}{\phi'(a)}\cdot f(a)\,.$$

Suppose on the other hand that we have an osculatory quadrature formula and the conditions of Corollary 2 are satisfied, then

(i) when the end point is not an abscissa we may take the angles of the arcs to be any angles less than π (or β when $f(z)$ has an essential singularity at an end point) and the contribution to the remainder from the arcs tends to zero with the radius of the arc;

(ii) when the end point, c (say), is an abscissa we must take semi-circular arcs above and below c and consider them simultaneously; the contribution to the remainder term from the arcs is then given by the expression (2.3.18).

2.4 Special Cases

We have so far confined our discussion of the contours C^+ and C^- to what can happen near the end points of the interval of integration. The formulae with which we have been concerned are of the types satisfying Corollary 1 or Corollary 2.

When only the conditions of the fundamental theorem are satisfied it will be necessary to examine the functions $\psi(z)$ and $\phi(z)$ on their own merits.

To discuss the remaining parts of the contours more information about the particular quadrature rule is required.

We will now discuss how we may derive the required contour integral expression of the remainder in a few special cases.

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Particular regard will be paid to the behaviour of the contours at the ends of the interval of integration.

This Section is divided into several parts.

In these parts we will obtain, by a suitable choice of the functions $\psi(z)$ and $\varphi(z)$, the most important Gaussian formulae, Section 2.4(a), and the formulae of Newton-Cotes, Section 2.4(b).

In the case of the Newton-Cotes formulae the end points of the interval are abscissae. We shall see in this case that the choice of the slopes at the end points is most important.

The Gaussian and Newton-Cotes formulae are of the type which satisfy Corollary 1 of Chapter I. However the repeated trapezoidal rule, Section 2.4(c), may be obtained directly from the theorem. We shall investigate this rule in some detail.

The Section concludes with a discussion of osculatory quadrature formulae in Section 2.4(d), and formulae of Obreschkoff type (see Salzer [21]) in Section 2.4(e).

2.4(a) Gaussian Quadrature Formulae

The quadrature formulae of Gaussian type are obtained from the consideration of a set of polynomials, $p_n(x)$ (say), of degree n which are orthogonal over a real interval $[a_1, b_1]$ with respect to a weight function $\omega(x)$. Thus the polynomials $p_n(x)$ satisfy the orthogonality relation

$$\int_{a_1}^{b_1} \omega(x)\, p_n(x)\, p_m(x)\, dx = \begin{cases} h_n , & m = n , \\ 0 , & m \neq n . \end{cases} \tag{2.4.1}$$

where h_n is a constant depending on n .

The quadrature formulae obtained from these polynomials are usually used when the interval, $[a_1, b_1]$, is the interval of integration $[a, b]$. The abscissae of the formula are the zeros of the polynomial $p_n(x)$ and these are interior points of the interval $[a_1, b_1]$.

Let us then identify the function $\phi(z)$ with the polynomial $p_{n+1}(z)$ where, for real values of z, $p_{n+1}(z) = p_{n+1}(x)$.

Now the weight function $\omega(x)$ may have singularities at the points a_1 and b_1 , e.g., in the Gauss-Chebyshev quadrature rule the weight function over the interval $[-1, 1]$ is $(1 - x^2)^{1/2}$ Therefore $\omega(x)\, \phi(x)$ will usually satisfy the Hölder condition, see equation (1.2.13), on (a_1, b_1) only.

There is no real difficulty when the interval is infinite. We could first take the end point of the interval to be finite and let it tend to infinity along the real axis. In the case of an infinite interval the weight function of the Gauss type formula is usually such that the condition (1.2.16) of Corollary 1 is satisfied immediately.

The cut (c, d) for the function $\psi(z)$ does then coincide with the interval (a, b). If we further require that $\psi(z)$ tends to zero as $|z|$ becomes large we have from Corollary 1

(2.4.2) $$\psi(z) = \int_a^b \frac{\omega(x)\, p_{n+1}(x)\, dx}{z - x} .$$

The coefficients $\lambda_{k,n}$, $k = 0(1)n$, of the quadrature formula from equation (1.2.9) are given by

(2.4.3) $$\lambda_{k,n} = - \frac{\psi(x_{k,n})}{p'_{n+1}(x_{k,n})} .$$

The quantities $\lambda_{k,n}$ defined by equation (2.4.3) are of course the well-known coefficients of the Gauss-type formula, see e.g. Kopal [32, Chapt.VII] .

By choosing each set of polynomials we thus obtain from the fundamental theorem (or Corollary 1) an expression for the remainder of each Gaussian formula in the required form of a contour integral. Contour integral expressions have been obtained in the cases of the Gauss-Jacobi, Gauss-Hermite and Gauss-Laguerre quadrature by Barrett [19] and MacNamee [16] . Their expressions were however derived under the assumption that the function $f(z)$ has no singularities on the interval $[a, b]$. Barrett attempts to deal with a branch singularity at the end points but his contour [19, Fig. 1.1], as we have pointed out in the Introduction, is wrongly chosen to cross the cut $[a, b]$. Our form of the remainder allows algebraic singularities and essential singularities at the end point.

Since the functions $\psi(z)$ and $\varphi(z)$ satisfy the conditions of Corollary 1, the behaviour of the contours C^+ and C^- at the end points is precisely that discussed in Section 2.3 of this chapter. Now the end points a and b of the interval are not abscissae of the quadrature formula. Thus from Section 2.3 the contribution from an arc at an end point will tend to zero with the radius of the arc. The angle of the arc we may then take to be any angle less than π or less than an angle β defined by a possible essential singularity of $f(z)$ at a.

For completeness we shall give the Gauss-Jacobi, Gauss-Laguerre and Gauss-Hermite quadrature rules with the remainder terms expressed as contour integrals.

Gauss-Jacobi Quadrature

In Gauss-Jacobi quadrature the polynomials $p_{n+1}(x)$ are the

Jacobi polynomials $P_{n+1}^{(\alpha,\beta)}(x)$, $n = 0, 1, 2, \ldots$. The polynomials are orthogonal over the interval $[-1, 1]$ with respect to the weight function $(1-x)^{\alpha}(1+x)^{\beta}$. If we denote by $\Pi_{n+1}^{(\alpha,\beta)}(z)$ the function $\psi(z)$ we have from equation (2.4.2)

$$\Pi_{n+1}^{(\alpha,\beta)}(z) = \int_{-1}^{1} \frac{(1-x)^{\alpha}(1+x)^{\beta} P_{n+1}^{(\alpha,\beta)}(x)}{z-x}\, dx . \tag{2.4.4}$$

The abscissae of the quadrature formula are the $(n+1)$ zeros of $P_{n+1}^{(\alpha,\beta)}(z)$. The quadrature formula may then be written

$$\int_{-1}^{1} (1-x)^{\alpha}(1+x)^{\beta} f(x)\, dx = \sum_{k=1}^{n} \lambda_{k,n} f(x_{k,n}) + R_{n+1}(f) \tag{2.4.5}$$

where

$$\lambda_{k,n} = - \frac{\Pi_{n+1}^{(\alpha,\beta)}(x_{k,n})}{P_{n+1}^{(\alpha,\beta)\prime}(x_{k,n})} , \tag{2.4.6}$$

for $k = 0(1)n$. From Theorem 1 and its corollary the remainder term is given by

$$R_{n+1}(f) = \frac{1}{2\pi i} \left\{ \int_{C^+} + \int_{C^-} \right\} \frac{\Pi_{n+1}^{(\alpha,\beta)}(z)}{P_{n}^{(\alpha,\beta)}(z)} f(z)\, dz . \tag{2.4.7}$$

The contours C^+ and C^- are of the type considered in the fundamental theorem except that the conditions on the slopes at the end points $+1$ and -1 are not as restrictive. For example we may let the slope of C^+ at -1 lie between π and 0 when $f(z)$ does not have an essential singularity at -1 or between π and $\pi-\beta'$ when $f(z)$ does have an essential singularity there. The contribution from the resulting arc as we have shown above tends to zero with the radius of the arc.

Gauss-Laguerre

The generalised Laguerre polynomials $L_{n+1}^{(\alpha)}(x)$, $n = 0, 1, 2, \ldots,$ $\alpha > -1$, are orthogonal over the semi-infinite interval $(0, \infty)$ with respect to the weight function $e^{-x} x^{\alpha}$. We see that the extra condition imposed on Corollary 1 when the interval is infinite is readily satisfied for any n. If then we denote by $\Lambda_{n+1}^{(\alpha)}(z)$ the function $\psi(z)$ we have,

(2.4.8) $$\Lambda_{n+1}^{(\alpha)}(z) = \int_0^{\infty} \frac{e^{-x} x^{\alpha} L_{n+1}^{\alpha}(x)}{z - x} f(x)\, dx .$$

The corresponding quadrature rule is given by

$$\int_0^\infty e^{-x} x^\alpha f(x)\,dx = \sum_{k=0}^{n} \lambda_{k,n} f(x_{k,n}) + R_{n+1}(f) \tag{2.4.9}$$

where

$$\lambda_{k,n} = \frac{\Lambda^{(\alpha)}_{n+1}(x_{k,n})}{L^{(\alpha)\prime}_{n+1}(x_{k,n})}\,, \tag{2.4.10}$$

for $k = 0(1)n$ and the points $x_{k,n}$, $k = 0(1)n$, are the zeros of the Laguerre polynomial. The remainder term is given by

$$R_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} \frac{\Lambda^{(\alpha)}_{n+1}(z)}{L^{(\alpha)}_{n+1}(z)} f(z)\,dz\,. \tag{2.4.11}$$

The behaviour of C^+ and C^- at the end point 0 is that described in Section 2.3 of this chapter. At the end point ∞ we need not concern ourselves with the behaviour of the contour there. We may simply consider the contours to be asymptotic to the positive real axis for large $|z|$.

A formula closely related to the Laguerre polynomials was stated by Barrett [19]. Barrett noted that the kth zero of the Laguerre polynomial is asymptotically equal to that of the Bessel function $J_\alpha(K^{\frac{1}{2}} x^{\frac{1}{2}})$ where $K = 4n + 2\alpha + 2$. This function is used in conjunction with the process described in Section 0.4

of the Introduction to obtain a quadrature formula, which Barrett calls the Gauss-Bessel integration rule, with the remainder term expressed in terms of a contour integral.

This formula is readily obtained from Corollary 1. Let us put

(2.4.12) $$\phi(z) = z^{-\alpha/2} J_\alpha[(kz)^{1/2}]$$

and

(2.4.13) $$\omega(z) = z^{\alpha}$$

Now the function $\omega(x)\phi(x)$ satisfies the condition of Corollary 1 over the semi-infinite interval $(0, \infty)$ and we find that the function $\psi(z)$ is given by

(2.4.14) $$\psi(z) = \int_0^\infty \frac{x^{\alpha/2} J_\alpha[(kx)^{1/2}]}{z - x}\, dx .$$

In this special case the integral on the right may be written down explicitly. We find from Erdélyi et al [33, p. 225] that equation (2.4.14) gives us

(2.4.15) $$\psi(z) = -2\, e^{-i\pi\alpha/2} z^{\alpha/2} K_\alpha[(kz)^{1/2} e^{i\pi/2}]$$

where K_α is the modified Bessel function of the second kind.

On using standard properties of the Bessel functions the coefficients $\lambda_{k,\infty}$, $k = 0, 1, 2, \ldots$, of the integration rule may be written in the form

$$\lambda_{k,\infty} = \pi^2 x_{k,\infty}^{\alpha+1} \left\{ Y_\alpha\left[(K x_{k,\infty})^{\frac{1}{2}}\right]\right\}^2 . \tag{2.4.16}$$

Equation (2.4.16) differs from that given by Barret by a factor $K^{-\frac{1}{2}}$. However in a personal communication with Barret it was established that a typographical error had been made in his paper and that the above equation, equation (2.4.16), is the correct form.

Gauss-Hermite

When considering a doubly infinite interval we use the Hermite polynomials $H_{n+1}(x)$ which are orthogonal over $(-\infty, \infty)$ with respect to the weight function e^{-x^2}. The function $\psi(z)$ which satisfies the conditions of Corollary 1 we shall denote by $\eta_{n+1}(z)$. We have from equation (1.2.14)

$$\eta_{n+1}(z) = \int_{-\infty}^{\infty} \frac{e^{-x^2} H_{n+1}(x)}{z - x} dx . \tag{2.4.17}$$

The Gauss-Hermite quadrature formula may now be written

$$(2.4.18) \qquad \int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx = \sum_{k=0}^{n} \lambda_{k,n} f(x_{k,n}) + R_{n+1}(f)$$

where, for $k = 0(1)n$,

$$(2.4.19) \qquad \lambda_{k,n} = -\frac{\eta_{n+1}(x_{k,n})}{H'_{n+1}(x_{k,n})}\ ,$$

and

$$(2.4.20) \qquad R_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} \frac{\eta_{n+1}(z)}{H_{n+1}(z)} f(z)\,dz\ .$$

The contours C^+ and C^- are of the type considered in the main theorem. Their behaviour as they approach the end points of the infinite interval may be taken to be asymptotic to the positive and negative directions of the real axis.

Barrett [19] again uses asymptotic properties of the zeros of the classical polynomials $H_{n+1}(x)$ to obtain a formula which is simply the repeated trapezoidal rule over $(-\infty, \infty)$.

Let us put

$$(2.4.21) \qquad \phi(z) = -\sin(\kappa^{\frac{1}{2}} z),$$

(2.4.22) $$\omega(z) = 1 .$$

We see that there are infinitely many zeros of the function $\varphi(z)$ in $(-\infty, \infty)$ so that the quadrature sum will have infinitely many terms. Now if we choose the function $\psi(z)$ to satisfy the equation

(2.4.23) $$\psi(z) = \begin{cases} \pi e^{+iK^{1/2}z} , & Im(z) > 0 , \\ \pi e^{-iK^{1/2}z} , & Im(z) < 0 , \end{cases}$$

we see that the conditions of the fundamental theorem are immediately satisfied. The corresponding integration formula which has an infinite number of abscissae is then given by

(2.4.24) $$\int_{-\infty}^{\infty} f(x)\, dx = \frac{\pi}{K^{1/2}} \sum_{k=-\infty}^{\infty} f\left(\frac{k\pi}{K^{1/2}}\right) + R(f)$$

with

(2.4.25) $$R(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} - \frac{\pi e^{\pm iK^{1/2}z}}{\sin(K^{1/2}z)} f(z)\, dz$$

where the upper sign is taken along C^+ and the lower sign along C^- . The contours C^+ and C^- are of the same type as those for the Gauss-Hermite formula.

We shall later in this Section use the fact that the above functions satisfy the conditions of Corollary 1 to show how $\psi(z)$ may be obtained from equation (1.2.14).

2.4(b) The Formulae of Newton-Cotes

In the Newton-Cotes quadrature formulae the interval $[a, b]$ is finite and the weight function, $\omega(x)$, is equal to unity. The abscissae $x_{k,n}$, $k = 0(1)n$, are equally spaced in the interval of integration and the end points a and b are abscissae of the formula.

We may then take for the function $\phi(z)$ the polynomial $p_{n+1}(z)$ of degree $(n+1)$, whose zeros are the abscissae, defined by

$$p_{n+1}(z) = \prod_{k=0}^{n} \left(z - a - \frac{(b-a)}{n} . k \right) . \tag{2.4.26}$$

Suppose now that the cut for the function $\psi(z)$ coincides with the interval $[a, b]$ and that $\psi(z)$ tends to zero for large $|z|$. Then the conditions of Corollary 1 are satisfied by the functions $\phi(z)$ and $\psi(z)$.

If we denote the function $\psi(z)$ by $q_{n+1}(z)$ we thus have from equation (1.2.14)

$$(2.4.27) \qquad q_{n+1}(z) = \int_a^b \frac{p_{n+1}(x)\, dx}{z - x} \quad .$$

Corresponding to the functions $p_{n+1}(z)$ and $q_{n+1}(z)$, given by equations (2.4.26) and (2.4.27), we have from Theorem 1 and its Corollary the numerical integration formula, see equation (1.2.10),

$$(2.4.28) \qquad \int_a^b f(x)\, dx = \sum_{k=1}^{n-1} \lambda_{k,n}\, f\left[a + \frac{(b-a)}{n}k\right] + R_{n+1}^{\times}(f)$$

where, for $k = 1(1)\{n-1\}$,

$$(2.4.29) \qquad \lambda_{k,n} = - \frac{q_{n+1}\left[a + \frac{(b-a)}{n} \cdot k\right]}{p'_{n+1}\left[a + \frac{(b-a)}{n} \cdot k\right]} \quad .$$

The remainder term $R_{n+1}^{\times}(f)$ is given by

$$(2.4.30) \qquad R_{n+1}^{\times}(f) = \frac{1}{2\pi i} \left\{ \int_{C^+} + \int_{C^-} \right\} \frac{q_{n+1}(z)}{p_{n+1}(z)}\, f(z)\, dz$$

where C^+ and C^- are contours of the type considered in Theorem 1.

Equation (2.4.28) is not as it stands in the form of a Newton-Cotes quadrature rule. The contributions from the end points of the range are included in the remainder term $R_{n+1}^{\times}(f)$ (compare equation (1.2.11)).

Now since the functions $\psi(z)$ and $\phi(z)$ satisfy the conditions of Corollary 1 the behaviour of the contours C^+ and C^- is that described in Section 2.3 of this chapter.

Consider first the behaviour at the end point a. There are two cases to consider:

(1) when $f(z)$ tends to a unique finite limit as z tends to a in the sector $|arg(z-a)| < \pi$;

(2) when $f(z)$ tends to a unique finite limit as z tends to a in the sector $|arg(z-a)| < \beta$ where $\beta < \pi$.

<u>Case (1)</u>: Suppose that $f(z)$ tends to a unique finite limit $f(a)$ as z tends to a in $|arg(z-a)| < \pi$. Then we can take the arc $\gamma_a(\alpha)$ in Section 2.3 to have angle π. Let us also take a similar arc below a. Following Section 2.3 we see that the contribution from these arcs is given by $\lambda_{0,n} f(a)$, where

(2.4.31) $$\lambda_{0,n} = -\frac{q_{n+1}(a)}{p'_{n+1}(a)}.$$

Suppose that we can take a similar pair of semi-circular arcs at the end point b. Then we can rewrite the formula (2.4.28) in the form

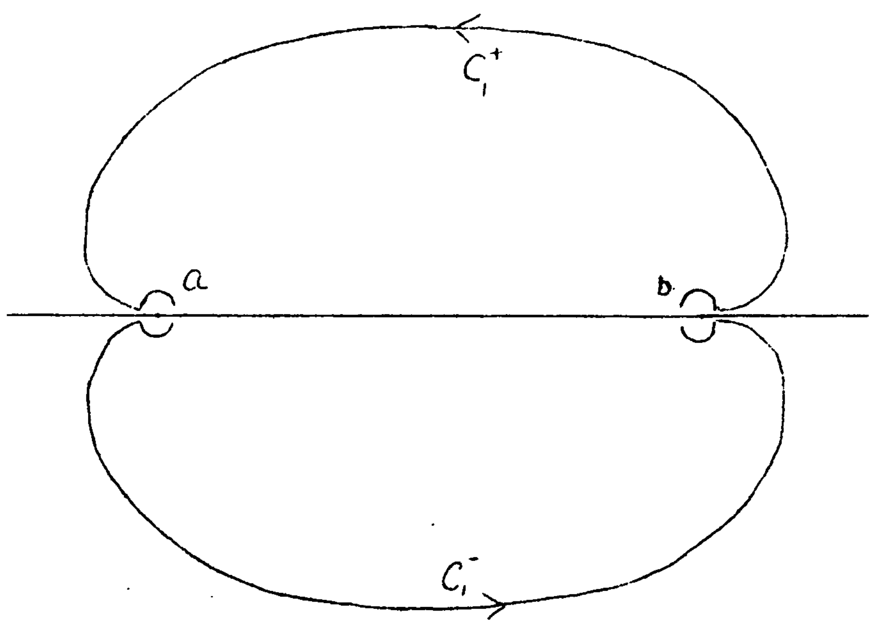
(2.4.32) $$\int_a^b f(x)\,dx = \sum_{k=0}^{n} \lambda_{k,n} f\left[a + \frac{(b-a)}{n}.k\right] + R_{n+1}(f)$$

where

$$(2.4.33) \qquad R_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{C_1^+} + \int_{C_1^-}\right\} \frac{q_{n+1}(z)}{p_{n+1}(z)} f(z)\, dz \,.$$

The contours C_1^+ and C_1^- satisfy the conditions imposed on the contours C^+ and C^- of Theorem 1 except that their slopes at the end points a and b have been changed by angles $\pm\pi$ to give the desired contribution to the quadrature sum on the right of equation (2.4.32). In fact C_1^+ is parallel to the positive direction of the real axis at its end points while C_1^- is parallel to the negative direction of the real axis there (see Fig. 2.2).

FIGURE 2.2



We now recognise equation (2.4.32) as the Newton-Cotes formula with the remainder in the required form of a contour integral.

Case (2): When $f(z)$ tends to a unique finite limit as z tends to a only along paths confined to the sector $|arg(z-a)| < \beta$, $\beta < \pi$, we cannot as in (1) above take semi-circles above and below a. However we can take an arc of angle (at most) β above a and the contribution to $R^{*}_{n+1}(f)$, from the expression (2.3.17), is then $-\frac{\beta}{2\pi} \lambda_{0,n} f(a)$. This is unfortunately only part of the required contribution to the quadrature sum.

In such cases it appears best to consider each function on its own merits.

For example let us consider the function $e^{-1/x}$ in the interval $(0,1)$. The limit as z tends to zero in $|arg(z)| < \pi/2$ is zero. Thus the contribution to the quadrature sum is zero and thus independent of the angle of the arc. We thus obtain the correct formula by allowing the contours C^{+} and C^{-} to approach and leave zero from the right of the imaginary axis.

So far the formulae we have considered are of interpolatory type, see e.g. Krylov [12, Chapt. 6]. The cut $[c, d]$ for the function $\psi(z)$ in each case coincides with the interval of integration $[a, b]$ and were determined from equation (1.2.14) of Corollary 1.

We shall now consider an extremely important case in which the interval $[c, d]$ is not simply the interval of integration.

2.4(c) The Repeated Trapezoidal Rule

In Section 2.4(a) when considering the Gauss-Hermite quadrature formula we obtained a quadrature rule which could be interpreted as a repeated trapezoidal rule over the doubly infinite interval $(-\infty, \infty)$. We shall now obtain an expression in terms of a contour integral for the error in the repeated trapezoidal rule over a finite interval. It will be shown how this expression gives us the well-known Abel-Plana and Euler-MacLaurin forms of the remainder, see e.g. Whittaker and Watson [34, p.145].

The remainder terms used by Goodwin [14] and MacNamee [16] are also readily obtained from this expression.

The process we shall use is no more than a slight generalisation of a well-known classical method, see e.g. Lindeloff [34, Chapt. III]. We describe this process here however to show how it fits into the structure of the fundamental theorem of Chapter I.

Let us take a more general form of the function $\phi(z)$ used in equation (2.4.21). Take

(2.4.34) $$\phi(z) = -\sin[\nu(z-a) - \lambda\pi]$$

where ν is a scaling factor (governing the tabular interval between the abscissae) and λ is a constant such that $0 \leq \lambda < 1$. The cut for the corresponding function $\psi(z)$ is the doubly infinite interval $(-\infty, \infty)$ and the weight function is the unit weight function.

From Corollary 1 we thus have

(2.4.35) $$\psi(z) = \int_{-\infty}^{\infty} \frac{-\sin[\nu(x-a) - \lambda\pi]}{z - x} dx .$$

Putting $y = \nu(x-a) - \lambda\pi$ in equation (2.4.35) we find

(2.4.36) $$\psi(z) = \int_{-\infty}^{\infty} \frac{-\sin y \, dy}{[\nu(z-a) - \lambda\pi] - y}$$

$$= \left\{ \int_{-\infty}^{0} + \int_{0}^{\infty} \right\} \frac{-\sin y \, dy}{[\nu(z-a) - \lambda\pi] - y} .$$

Substituting $y = t^{1/2}$, equation (2.4.36) becomes

(2.4.37) $$\psi(z) = \int_{0}^{\infty} \frac{-\sin t^{1/2} \, dt}{[\nu(z-a) - \lambda\pi]^2 - t} .$$

Finally from Erdélyi et al [35, p.219] we find that equation (2.4.37) gives

(2.4.38) $$\psi(z) = \begin{cases} \pi e^{+i[\nu(z-a)-\lambda\pi]}, & Im(z) > 0, \\ \pi e^{-i[\nu(z-a)-\lambda\pi]}, & Im(z) < 0, \end{cases}$$

Equation (2.4.38) agrees with the result one would expect from equation (2.4.23).

The quadrature formula is then given by

(2.4.39) $$\int_a^b f(x)\,dx = \sum_k \frac{\pi}{\nu} f\left[a + (k+\lambda)\frac{\pi}{\nu}\right] + R^x(f)$$

where $\sum_k$ denotes a sum taken over the abscissae interior to the interval $[a, b]$. If either of the end points is an abscissa the contribution to the quadrature sum from the end point is included in the remainder term $R^x(f)$.

From the fundamental theorem the remainder term in equation (2.4.39) is then given by

(2.4.40) $$R^x(f) = \frac{1}{2\pi i}\int_{C^+} - \frac{\pi e^{+i[\nu(z-a)-\lambda\pi]}}{\sin[\nu(z-a)-\lambda\pi]} f(z)\,dz + $$
$$+ \frac{1}{2\pi i}\int_{C^-} - \frac{\pi e^{-i[\nu(z-a)-\lambda\pi]}}{\sin[\nu(z-a)-\lambda\pi]} f(z)\,dz$$

where the contours C^+ and C^- are of the type considered in the fundamental theorem.

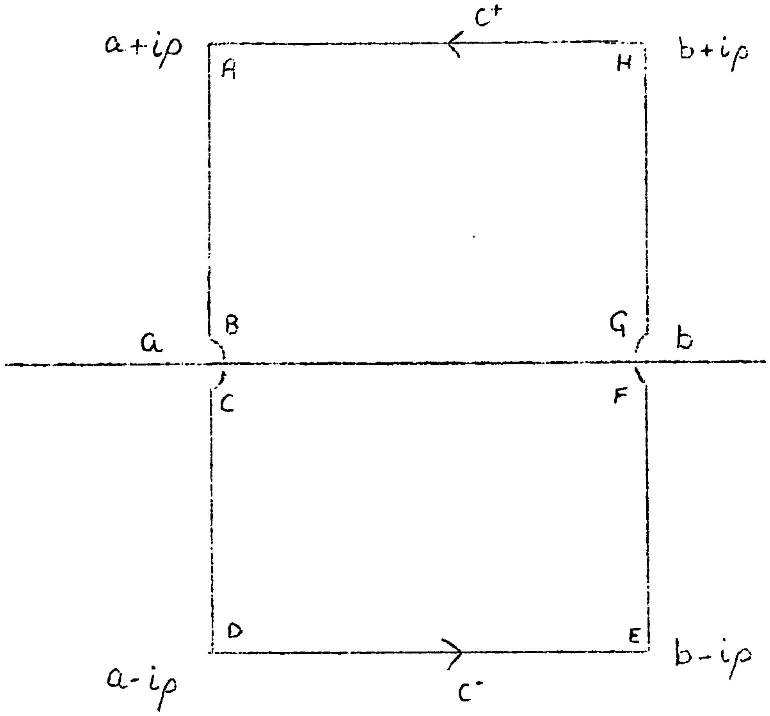
By choosing suitably the parameters γ and λ and the contours C^+ and C^- the Abel-Plana and Euler-MacLaurin forms of the remainder may now be obtained. We can also obtain from equation (2.4.40) the results used by both MacNamee [16] and Goodwin [14] .

The Rectangular Contour

Suppose first that $f(z)$ tends to a unique limit, $f(a)$ (say), as z tends to a for $|\arg(z-a)| \leq \pi/2$. We can therefore let the contours C^+ and C^- approach the end point along any path in the sector $|\arg(z-a)| \leq \pi/2$. Let us take the angle α of the small arc at a to be $\pi/2$ with a similar arc below a . Suppose that the behaviour at the end point b is similar.

Let us now take the remaining part of C^+ to consist of straight lines at a and b parallel to the imaginary axis and the line through the points $a+i\rho$ and $b+i\rho$, $\rho>0$, parallel to the real axis. Let us take the contour C^- to be of a similar shape below the real axis, see Fig. 2.3.

FIGURE 2.3



The functions $\psi(z)$ and $\phi(z)$ satisfy the conditions of Corollary 1 and hence the behaviour of the contours at the end points a and b follow that described in Section 2.3. Thus the contribution to the remainder term from the integral around the arc $\gamma_a(\pi/2)$ as the radius of the arc tends to zero is either zero or equal to, when the end point is an abscissa, $\pi/\nu \cdot \frac{1}{4} f(a)$. The non-zero contribution would be added to the quadrature sum.

Similar results hold for the arc below a and the arcs above and below b .

The remainder term $R(f)$ which does <u>not</u> contain the contribution from the end points (see equation (1.2.11)) is, then, given by the integrals along the edges of the rectangular contour. Let us label the points on the rectangle as shown in Fig. 2.3. Also let us denote by AB the line from $a+i\rho$ to a and denote by $R(f,AB)$ the contribution to the remainder term, $R(f)$, from the integral along AB.

Now on AB, $z = a+iy,\ \rho \geq y > 0$. Therefore from equation (2.4.40) we have immediately,

$$\text{(2.4.41)} \qquad R(f,AB) = \frac{1}{i}\int_0^\rho \frac{f(a+iy)\ dy}{e^{(2\nu y+2\lambda\pi i)}-1} .$$

Similarly,

$$\text{(2.4.42)} \qquad R(f,CD) = -\frac{1}{i}\int_0^\rho \frac{f(a-iy)\ dy}{e^{(2\nu y-2\lambda\pi i)}-1} ,$$

$$\text{(2.4.43)} \qquad R(f,DE) = -\int_a^b \frac{f(x-i\rho)\ dx}{e^{2\rho\nu}e^{2i[\nu(x-a)-\lambda\pi]}-1} ,$$

$$\text{(2.4.44)} \qquad R(f,EF) = -\frac{1}{2}\int_0^\rho \frac{e^{-\nu y}\ e^{-i[\nu(b-a)-\lambda\pi]}}{\sin[\nu(b-a-iy)-\lambda\pi]} f(b-iy)\ dy ,$$

$$\text{(2.4.45)} \qquad R(f,GH) = -\frac{1}{2}\int_0^\rho \frac{e^{-\nu y}\ e^{+i[\nu(b-a)-\lambda\pi]}}{\sin[\nu(b-a+iy)-\lambda\pi]} f(b-iy)\ dy$$

and

(2.4.46) $$R(f, HA) = -\int_a^b \frac{f(x+i\rho)\,dx}{e^{2\rho\nu}e^{-2i[\nu(x-a)-\lambda\pi]}-1} .$$

The Abel-Plana Form of the Remainder

Let us choose $\lambda = 0$ and divide the interval $[a, b]$ into n equal parts, tabular interval h. The end points a and b are abscissae of the formula and the integrals around the arcs of the circles at the end points contribute to the quadrature sum amounts $-h/2 \cdot f(a)$ and $h/2\, f(b)$ respectively.

Thus the integration formula may be written

(2.4.47) $$\int_a^b f(x)\,dx = h \sum_{k=0}^{n}{}'' f(a+kh) + R_{n+1}(f)$$

where $\sum''$ denotes a sum whose first and last terms are halved.

The remainder term $R_{n+1}(f)$ is the sum of the six terms given by equations (2.4.41)-(2.4.46) with $\lambda = 0$ and $\nu = \pi/h$

If we now assume that $f(z)$ is analytic and bounded in the strip $a \le Re(z) \le b$ then it is readily shown that $R(f, DE)$ and $R(f, HA)$ tend to zero as ρ tends to infinity.

On combining the remaining four integrals we obtain the Abel-Plana form of the remainder given by

(2.4.48) $$R_{n+1}(f) = -\frac{1}{i}\int_0^\infty \frac{f(b+iy) - f(b-iy) - f(a+iy) + f(a-iy)}{e^{2\pi y/h} - 1}\,dy .$$

The Euler-MacLaurin Form of the Remainder

The Euler-MacLaurin form of the remainder may be obtained directly from equation (2.4.48) as follows.

Let us expand each of the functions appearing in the integral on the right of equation (2.4.48) in its Taylor series, for example we may write

$$f(b+iy) = f(b) + (iy)f'(b) + \frac{(iy)^2}{2!}f''(b) + \cdots \quad (2.4.49)$$

Then equation (2.4.48) becomes

$$R_{n+1}(f) = -\frac{1}{i}\int_0^\infty \frac{\left\{\left[(iy)f'(b) + \frac{(iy)^3}{3!}f'''(b) + \cdots\right] - \left[(iy)f'(a) + \frac{(iy)^3}{3!}f'''(a) + \cdots\right]\right\}}{e^{2\pi y/h} - 1}\,dy \,. \quad (2.4.50)$$

Using the result, see Abramowitz and Stegun [35, equations (23.2.7) and (23.2.16)]

$$4r\int_0^\infty \frac{y^{2r-1}}{e^{2\pi y}-1}\,dy = (-1)^{r-1}B_{2r} \quad (2.4.51)$$

where B_{2r} is the $2r$th Bernoulli number, equation (2.4.51) becomes

$$R_{n+1}(f) = \sum_{r=1}^{\infty} \frac{(-1)^r h^{2r} B_{2r}}{2r!}\left[f^{(2r-1)}(b) - f^{(2r-1)}(a)\right] . \quad (2.4.52)$$

Equation (2.4.52) is of course the Euler-MacLaurin form of the remainder.

It should be noted that equation (2.4.52) only holds when the infinite series converges: if not we must truncate the series after a finite number of terms with an appropriate remainder term.

Extension to Functions with Algebraic Singularities at the End Points

The Euler-MacLaurin formula was extended to functions with algebraic singularities by Navot [3] . This extension was later generalised by Ninham and Lyness [5] . The formulae obtained by these authors are readily obtained using the contour integral form of the remainder term.

Consider the interval $[0, 1]$ and let us take as an example the function $f(z)$ to be of the form

(2.4.53) $$f(z) = z^{\alpha} g(z)$$

where $\alpha \geq 0$ and $g(z)$ is analytic at $z = 0$. We have chosen $\alpha \geq 0$ so that we can use an integration formula in which the end point is an abscissa. We recall that the function must be defined at an abscissa for the quadrature sum to have any meaning. Both Ninham and Lyness, and Navot consider α in the range, $0 \geqslant \alpha > -1$, in which case the integration formula must not have an abscissa at $z=0$. The following methods are readily adapted to treat such a case.

Since $f(z)$ has a branch point at the origin we may cut the complex plane along the negative real axis and take the rectangular contour depicted in Fig. 2.3.

The function $f(z)$ tends to a unique limit in $|\arg(z)| < \pi$ and we may therefore follow the discussion of the Abel-Plana formula. Thus equation (2.4.48) gives us

$$R_{n+1}(f) = i\int_0^\infty \frac{f(1+iy)-f(1-iy)}{e^{2\pi y/h}-1}\,dy - i\int_0^\infty \frac{f(iy)-f(-iy)}{e^{2\pi y/h}-1}\,dy \,. \tag{2.4.54}$$

From the above discussion of the Euler-MacLaurin formula the first integral on the right of equation (2.4.54) gives us

$$i\int_0^\infty \frac{f(1+iy)-f(1-iy)}{e^{2\pi y/h}-1}\,dy = \sum_{r=1}^\infty \frac{(-1)^r h^{2r} B_{2r}}{(2r)!} f^{(2r-1)}(1) \tag{2.4.55}$$

We cannot however apply this result to the second integral. On the other hand we may write

$$\begin{aligned} f(iy) &= (iy)^\alpha g(iy) \\ &= (iy)^\alpha g(0) + (iy)^{\alpha+1} g'(0) + \frac{(iy)^{\alpha+2}}{2!} g''(0) + \cdots \,. \end{aligned} \tag{2.4.56}$$

Substituting equation (2.4.56) into the second integral on the right of equation (2.4.53) we obtain

$$(2.4.57) \quad -i\int_0^\infty \frac{f(iy)-f(-iy)}{e^{2\pi y/h}-1}\,dy = -i\int_0^\infty \left\{ \frac{y^\alpha g(0)[i^\alpha-(-i)^\alpha]}{e^{2\pi y/h}-1} + \frac{y^{\alpha+1} g'(0)[i^{\alpha+1}-(-i)^{\alpha+1}]}{e^{2\pi y/h}-1} + \right\} dy$$

Now from Abramowitz and Stegun [35, p.807] we have

$$(2.4.58) \quad \frac{1}{\Gamma(s)}\int_0^\infty \frac{x^{s-1}}{e^x-1}\,dx = 2^s \pi^{s-1} \sin(\tfrac{1}{2}\pi s)\,\Gamma(1-s)\,\zeta(1-s)$$

where $\zeta(s)$ is the Riemann-zeta function.

Using the continuation formula for the Γ-functions equation (2.4.58) may be written

$$(2.4.59) \quad \int_0^\infty \frac{x^{s-1}}{e^x-1}\,dx = \frac{2^{s-1}\pi^s \zeta(1-s)}{\cos(\pi s/2)}$$

Using equation (2.4.59), equation (2.4.57) now gives us

$$(2.4.60) \quad -i\int_0^\infty \frac{f(iy)-f(-iy)}{e^{2\pi y/h}-1}\,dy = -\sum_{r=0}^{\infty}\left(\frac{h}{2\pi}\right)^{\alpha+r+1}(2\pi)^{\alpha+r+1}\zeta(-\alpha-r)\,\frac{g^{(r)}(0)}{r!}\,.$$

Substituting equation (2.4.55) and (2.4.60) into equation (2.4.54) we find

$$R_{n+1}(f) = \sum_{r=1}^{\infty} \frac{(-1)^r h^{2r} B_{2r}}{2r!} f^{(2r-1)}(1) - \sum_{r=0}^{\infty} h^{\alpha+r+1} \zeta(-\alpha-r) \cdot \frac{g^{(r)}(0)}{r!} . \tag{2.4.61}$$

Again the infinite sums are asymptotic and must be terminated after a finite number of terms with an appropriate remainder term. The equation (2.4.61) is a special case of the equation obtained by Ninham and Lyness [5, equation 78] . The above methods are readily extended to functions of a more general form.

MacNamee's Expression

MacNamee [16] is concerned with the application of the repeated trapezoidal rule to the approximate evaluation of integrals of the form

$$\mathcal{I}_1 = \int_0^{\infty} f(x)\, dx . \tag{2.4.62}$$

So that the integral (2.4.62) may converge it is necessary that

$$\lim_{x \to \infty} f(x) = 0 . \tag{2.4.63}$$

To obtain MacNamee's expression for the remainder we take (in equations (2.4.41)-(2.4.46)) the point a as the origin and let b tend to infinity along the positive real axis. As we let b tend to infinity the number of abscissae in the interval (a, b) tends to infinity also. Let us again take the parameter $\nu = \pi/h$ and include the contribution from the arcs at the end points in the quadrature sum.

We may then write the quadrature formula in the following way

$$(2.4.64) \quad \int_0^\infty f(x)\,dx = h \sum_{k=0}^{\infty} f[(k+\lambda)h] + R(f)$$

where the first term is halved when $\lambda = 0$, that is when the end point is an abscissa. The remainder term $R(f)$ is obtained from equations (2.4.41)-(2.4.46) on substituting the appropriate values for a, b and ν.

Now using equation (2.4.63) it is readily shown that $R(f, EF)$ and $R(f, GH)$, given by equations (2.4.44) and (2.4.45) respectively, tend to zero as b tends to infinity. Thus the remainder term, $R(f)$, in equation (2.4.45) is the sum of the contributions $R(f, AB)$, $R(f, CD)$, $R(f, DE)$ and $R(f, HA)$.

As we have pointed out in Section 0.3 MacNamee considers the remainder term in two parts a correction term, $C(\lambda, h, \rho)$, which is the contribution from the lines AB and CD and an error term, $E(\lambda, h, \rho)$, from the lines DE and HA. From equations (2.4.41) and (2.4.42) we thus have

$$(2.4.65) \quad C(\lambda,h,\rho) = -\tfrac{1}{2}\int_0^\rho \frac{[f(iy)-f(-iy)]\,[\cos(2\lambda\pi)-e^{-2\pi y/h}]}{[\cos(2\pi y/h)-\cos(2\lambda\pi)]}\,dy -$$

$$-\sin(2\lambda\pi/h)\int_0^\rho \frac{f(iy)+f(-iy)}{\cos(2\pi y/h)-\cos 2\lambda\pi}\,dy .$$

The error term $E(\lambda,h,\rho)$ from equations (2.4.43) and (2.4.46) is given by

$$(2.4.66) \quad E(\lambda,h,\rho) = -\int_0^\infty \frac{f(x+i\rho)\,.\,dx}{e^{2\rho\pi/h}e^{-2i(\pi x/h-\lambda\pi)}-1} - \int_0^\infty \frac{f(x-i\rho)\,.\,dx}{e^{2\rho\pi/h}e^{2i(\pi x/h-\lambda\pi)}-1} .$$

The expression given by equations (2.4.65) and (2.4.66) are the expressions used by MacNamee [16] in his analysis.

Goodwin's Result

The case of the doubly infinite interval $(-\infty,\infty)$ is discussed by Goodwin [14] . Goodwin discusses the remainder term when the repeated trapezoidal rule is used to evaluate integrals of the form

$$\mathcal{J}_2 = \int_{-\infty}^{\infty} e^{-x^2} f(x)\, dx . \tag{2.4.67}$$

It is assumed that the function $f(x)$ is an even function, that is,

$$f(x) = f(-x) . \tag{2.4.68}$$

From equation (2.4.68) we have immediately

$$2\int_{0}^{\infty} e^{-x^2} f(x)\,dx = \int_{-\infty}^{\infty} e^{-x^2} f(x)\, dx . \tag{2.4.69}$$

If we take $\lambda = 0$ in equations (2.4.65) and (2.4.66) and use equations (2.4.68) and (2.4.69) we have

$$R(f) = -2\int_{-\infty}^{\infty} \frac{e^{-x^2} f(x+i\rho)}{e^{2\rho\pi/h} e^{-2i\pi x/h} - 1}\, dx . \tag{2.4.70}$$

Goodwin makes use of equation (2.4.70) to obtain some extremely useful estimates of the remainder term for some special functions.

2.4(d) Osculatory Quadrature Formulae

We have shown in Theorem 2 of Chapter I how an expression for the remainder in terms of a contour integral may be obtained for osculatory quadrature formulae. We shall now discuss the integration formula derived from the Hermite interpolation formula.

In the Hermite interpolation formula we require that the value of the function and its first derivative agree with the value of the Hermite interpolatory polynomial and its derivative at each of the $(n+1)$ points, $x_{k,n}$, $k = 0(1)n$.

Let us write

$$\pi(x) = (x - x_{0,n})(x - x_{1,n}) \ldots (x - x_{n,n}) \tag{2.4.71}$$

and put

$$l_k(x) = \frac{\pi(x)}{(x - x_{k,n})\pi'(x_{k,n})} \tag{2.4.72}$$

Then the Hermite interpolation formula may be written, see Hamming [2, p.96],

$$f(x) = \sum_{k=0}^{n} h_{k,0,n}(x) f(x_{k,n}) + \sum_{k=0}^{n} h_{k,1,n}(x) f'(x_{k,n}) + \\ + r_{2n+2}(f) \tag{2.4.73}$$

where

(2.4.74) $$h_{k,0,n} = \left[1 - 2\,\ell_k'(x_{k,n})(x - x_{k,n})\right]\left[\ell_k(x)\right]^2$$

and

(2.4.75) $$h_{k,1,n} = (x - x_{k,n})\left[\ell_k(x)\right]^2.$$

The quantity $r_{2n+2}(f)$ is the remainder of the interpolation formula.

To obtain the corresponding integration formula we multiply each side of equation (2.4.73) by the weight function $\omega(x)$ and integrate between the limits a and b. Thus

(2.4.76) $$\int_a^b \omega(x) f(x)\,dx = \sum_{k=0}^{n} \lambda_{k,0,n} f(x_{k,n}) + \sum_{k=0}^{n} \lambda_{k,1,n} f'(x_{k,n}) + R_{2n+2}(f)$$

where

(2.4.77) $$\lambda_{k,0,n} = \int_a^b \omega(x)\, h_{k,0,n}\,dx$$

and

$$\lambda_{k,1,n} = \int_a^b \omega(x)\, h_{k,1,n}(x)\, dx \quad . \tag{2.4.78}$$

$R_{2n+2}(f)$ is the remainder term of the integration rule.

To express the remainder term $R_{2n+2}(f)$ in terms of a contour integral we make use of the second theorem of Chapter I and Corollary 2. Let us take the function $\phi(z)$ to be defined by

$$\phi(z) = [\pi(z)]^2 \tag{2.4.79}$$

where the points $x_{k,n}$, $k = 0(1)n$ are interior points of the interval $[a,b]$.

Then if we take the cut for the corresponding function $\psi(z)$ to be the interval $[a,b]$ and require that $\psi(z)$ tends to zero as $|z|$ tends to infinity we see that the conditions of Corollary 2 are satisfied. Thus we may write

$$\psi(z) = \int_a^b \frac{\omega(x)\,\phi(x)}{z-x}\, dx \quad . \tag{2.4.80}$$

From equation (1.3.16) with $p = 2$, the weight factors are given by

$$\lambda_{k,r,n} = -\frac{\binom{2-1}{r}}{r!}\, \frac{d^{1-r}}{dz^{1-r}}\left[(z-x_{k,n})^2\, \frac{\psi(z)}{\phi(z)}\right]_{z=x_{k,n}} \tag{2.4.81}$$

for $r = 0, 1$ and $k = 0(1)n$. Equations (2.4.81) may be written in the form

(2.4.82) $$\lambda_{k,0,n} = -2\,\frac{\psi'(x_{k,n})}{\varphi''(x_{k,n})} + \frac{2}{3}\,\frac{\psi(x_{k,n})\,\varphi'''(x_{k,n})}{[\varphi''(x_{k,n})]^2}$$

and

(2.4.83) $$\lambda_{k,1,n} = -\,\frac{2\,\psi(x_{k,n})}{\varphi''(x_{k,n})} ,$$

for $k = 0(1)n$.

Using equations (2.4.79) and (2.4.80) it is easily shown that equations (2.4.82) and (2.4.83) are equivalent to equations (2.4.77) and (2.4.78) respectively.

From Theorem 2 the remainder term $R_{2n+2}(f)$ in equation (2.4.76) is then given by

(2.4.84) $$R_{2n+2}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} \frac{\psi(z)}{\varphi(z)}\, f(z)\, dz$$

where the contours are of the type considered in the fundamental theorem.

Since the functions $\psi(z)$ and $\varphi(z)$ satisfy the conditions of Corollary 2 the behaviour of the contours C^+ and C^-

at the end points a and b follows that discussed in Section 2.3(a).

Consider the end point a .

Let us suppose that $f(z)$ tends to a unique limit as z tends to a in the sector $|\arg(z-a)| < \beta$. Then because a is not an abscissa the contribution from the arcs at the end point is zero. We may then allow the contours C^+ and C^- to approach a along any path confined to this sector.

When the end point is an abscissa the remainder term given by equation (2.4.84) includes the contribution from the end point $a = x_{0,n}$ (say). To choose any angle other than that required in the fundamental theorem we must have that $f(z)$ and $f'(z)$ tend to unique limits $f(a)$ and $f'(a)$ respectively as z tends to a in the sector $|\arg(z-a)| < \pi$. To obtain the required contribution to the quadrature sum we take arcs of angle π above and below the end point a . From the expression (2.3.18) this contribution is given by

(2.4.85) $$\lambda_{0,0,n} f(a) + \lambda_{0,1,n} f'(a)$$

where the weight factors are those given by equations (2.4.82) and (2.4.83).

2.4(e) Obreschkoff type Quadrature Formulae

Obreschkoff type quadrature formulae make use of the function and its successive derivatives at only the end points of the range of integration. The formula may be written

$$\int_a^b f(x)\,dx = \sum_{r=0}^{p-1} \lambda_{0,r,2} f^{(r)}(a) + \sum_{r=0}^{p-1} \lambda_{1,r,2} f^{(r)}(b) + R_{2p}(f). \tag{2.4.86}$$

In this case we would take

$$\phi(z) = (z-a)^p (z-b)^p . \tag{2.4.87}$$

Let us now take the cut for the function $\psi(z)$ to be the interval $[a, b]$ and require that $\psi(z)$ tends to zero for large $|z|$. From Corollary 2 we then have

$$\psi(z) = \int_a^b \frac{(x-a)^p (x-b)^p}{z-x}\, dx . \tag{2.4.88}$$

The remainder term $R_{2p}^{\times}(f)$ which includes the contribution to the quadrature sum from the end points is then given by

$$R_{2p}^{\times}(f) = \frac{1}{2\pi i} \left\{ \int_{c^+} + \int_{c^-} \right\} \frac{\psi(z)}{\phi(z)} f(z)\, dz . \tag{2.4.89}$$

To establish the formula (2.4.86) suppose that $f(z)$ and its first $(p-1)$ derivatives tend to unique limits as z tends to a in the sector $|\arg(z-a)| < \pi$. Then following the arguments of Section 2.3(a) the contribution from the end points is given by the expression (2.3.18). We may treat the end point b similarly.

Equation (2.4.80) then becomes

$$R_{2p}^{X}(f) = \sum_{r=0}^{p-1} \lambda_{0,r,2}\, f^{r}(a) + \sum_{r=0}^{p-1} \lambda_{1,r,2}\, f^{(r)}(b) + R_{2p}(f) \tag{2.4.90}$$

where $R_{2p}(f)$, the required remainder term, is given by

$$R_{2p}(f) = \frac{1}{2\pi i}\left\{\int_{C_1^+} + \int_{C_1^-}\right\} \frac{\psi(z)}{\varphi(z)}\, f(z)\, dz \,. \tag{2.4.91}$$

The contours C_1^+ and C_1^- are of the type considered in the Newton-Cotes formula, see Fig. 2.2.

Summary

So far in this chapter we have discussed the behaviour of the contours C^+ and C^- near only the end points of the interval of integration. We have considered arcs of angle α

at the end points and have shown how in certain cases the contribution to the remainder term from the integral around this arc tends to zero. On the other hand when the end point is an abscissa the integral around the arc usually contributes to the quadrature sum by an amount depending on the angle of the arc. Care had to be taken in the osculatory quadrature case when the end point was an abscissa. To obtain a finite result for such a case an arc of angle π was chosen.

These results were then used in conjunction with the fundamental theorem to obtain an expression in terms of a contour integral for the remainder term when specific quadrature rules were applied to various classes of functions.

Before we proceed to the next chapter we will discuss a rather special case when the contours C^+ and C^- combine to form a single contour.

2.5 The Important Case of a Closed Contour

In certain important cases the contours C^+ and C^- combine to give a single closed contour surrounding the basic interval of integration $[a, b]$. Since we shall use such contours in our discussion of convergence in the following chapter,

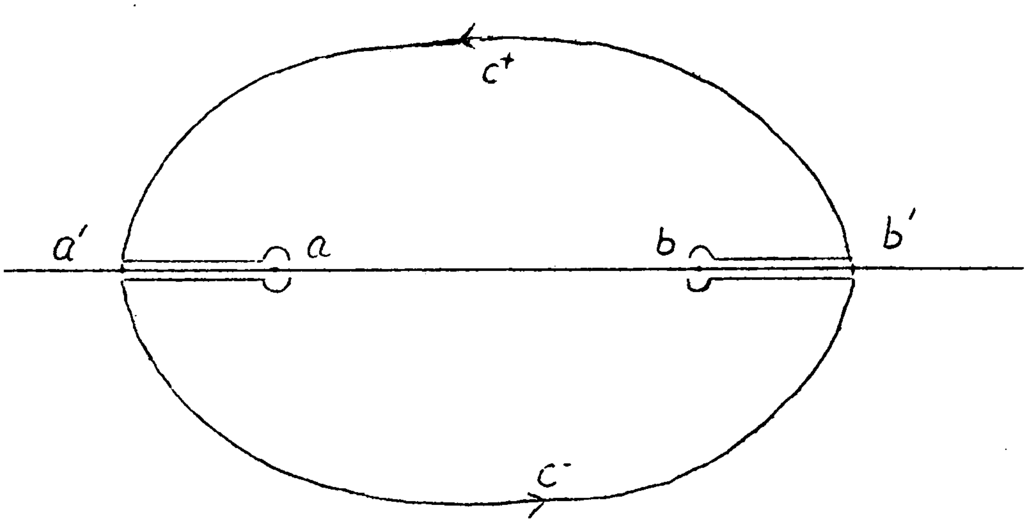
Chapter III, we shall now establish conditions under which we may take the contours to be a single closed contour.

Consider first the end point a and suppose that $f(z)$ does not have a singularity at a. Suppose further that the cut for the function $\psi(z)$ coincides with the interval of integration $[a, b]$.

Now let us take arcs of angle π above and below the end point a and let the radii of these arcs tend to zero. From our assumptions, Section 2.3 shows us that the contribution from the arcs is zero or contributes to the quadrature sum.

Now there is a point a' on the x-axis, such that $a' < a$, and such that the function $\psi(z) f(z)/\phi(z)$ has no singularities on the segment (a', a) of the real axis (all three functions $\psi(z)$, $\phi(z)$ and $f(z)$ have been chosen separately to satisfy this). Let part of C^+ and C^- lie along (a', a) above and below the real axis respectively, see Fig. 2.4.

FIGURE 2.4



The contribution to $R_{n+1}(f)$ from the integrals along those parts of C^+ and C^- lying along (a', a) cancel and we may therefore consider the contours C^+ and C^- to have been deformed into a single contour passing through a'.

If we can find a point b' which performs a similar role for the end point b as a' does for a then the single contour will become a closed contour surrounding the basic interval $[a, b]$. The remainder term may then be expressed in the form

$$R_{p(n+1)}(f) = \frac{1}{2\pi i} \int_C \frac{\psi(z)}{\varphi(z)} f(z)\, dz \tag{2.5.1}$$

where C is a closed contour surrounding the basic interval $[a, b]$ and lying in the region common to both D_1, the region in which $f(z)$ is analytic, and D_2, the region in which there are no zeros of $\varphi(z)$ other than those at the abscissa of the formula.

We see then that the remainder term reduces to the form of equation (2.5.1) when,

(1) the cut for $\psi(z)$ coincides with the interval, and

(2) $f(z)$ is analytic in the interval $[a, b]$.

CHAPTER III

THE CONVERGENCE OF QUADRATURE FORMULAE

3.1 Introductory Remarks on Convergence

The Quadrature Scheme

Consider the general osculatory quadrature formula, as given by equation (0.1.3), in the form

$$(3.1.1)\quad \int_a^b \omega(x) f(x)\,dx = \sum_{r=0}^{p-1} \sum_{k=0}^{n} \lambda_{k,r,n} f^{(r)}(x_{k,n}) + R_{(n+1)p}(f).$$

We shall mean by a quadrature scheme a sequence of formulae of the type given by equation (3.1.1) for either $n = 0, 1, 2, \ldots$ or $p = 0, 1, 2, \ldots$.

Convergence

A quadrature scheme will be said to converge if the remainder term, $R_m(f)$, in equation (3.1.1) tends to zero as m tends to infinity.

The main purpose of this thesis is not to give a detailed analysis of the convergence of quadrature schemes. However, a discussion of convergence arises naturally from an examination of asymptotic expressions for the ratio $\psi(z)/\phi(z)$ which occurs in the contour integral form of the remainder term which we obtained in Chapter I.

Asymptotic expressions for the ratio $\psi(z)/\phi(z)$ are unfortunately not always easy to obtain. We shall however, in this chapter, study the conditions under which certain well-known quadrature schemes converge. These conditions will, of course, depend on both the function and the quadrature scheme. We shall confine ourselves in this present discussion to functions which can be continued analytically into some region of the complex plane.

The convergence of quadrature schemes has been considered by many authors. According to Davis, see Todd [8] , Stieltjes first proved the convergence of the Gaussian quadrature scheme for the class of Riemann integrable functions in 1884.

The corresponding interpolation problem for equally spaced abscissae was considered by Runge in 1901. Runge, see Lanczos [36, p.348] , discovered that for such interpolation formulae quite 'wrong' results are obtained for very simple analytic functions.

This leads us to the Newton-Cotes quadrature scheme which is one of the most interesting and widely discussed schemes as far as convergence is concerned. The Newton-Cotes scheme does not converge even for functions which are analytic in a region of the complex plane which includes the interval of integration.

The following numerical example appears to indicate this. Let us take the interval of integration to be $[-1, 1]$ and consider the function $f(x) = 1/[(1/4)^2 + x^2]$. Now $f(z)$ is certainly analytic on $[-1, 1]$. However the Newton-Cotes scheme applied to $f(x)$ gives the following table of values, Table 3.1, which suggests that the quadrature scheme may not converge.

TABLE 3.1

n	$\sum_{k=0}^{n} \lambda_{k,n} f(x_{k,n})$	(actual) $R_{n+1}(f)$
2	21.9608	20.3900
6	13.3152	11.7444
14	18.3554	16.7846
16	- 1.2082	- 2.7790
18	29.1341	27.5633
20	-19.1007	-20.6715

A detailed examination of the coefficients in the Newton-Cotes scheme was made by Ouspensky [37] in 1925. He showed that the coefficients $\lambda_{k,n}$, $k = 2(1)\{n-2\}$, tend to infinity with n. The only conclusion which is then made by Ouspensky is that the Newton-Cotes scheme was of no practical use for large values of n.

In a more positive approach to the problem Polya [38] showed analytically that the Newton-Cotes scheme does not converge when applied to the function $f(x)$ given by

(3.1.2) $$f(x) = \sum_{\nu=0}^{\infty} \frac{a^{\nu!} \sin(\nu! \pi x)}{-\cos \pi x}, \quad \tfrac{1}{2} < a < 1.$$

The analytic continuation $f(z)$ of the function $f(x)$ into the complex plane is analytic in the strip $|Im(z)| < -\log a/\pi$. Polya obtained precisely the same asymptotic estimates of the coefficients $\lambda_{k,n}$, for large values of n, as Ouspensky, and used them to show that the quadrature sum $\sum_{k=0}^{n!} \lambda_{k,n!} f(x_{k,n!})$ tended to infinity with n.

Using the linear functional approach discussed in Section 0.2 of the Introduction, Davis, see Todd [8], shows however that the Newton-Cotes scheme may be applied successfully to functions which are analytic in a "sufficiently large" portion of the complex plane. Davis proceeds in the following way.

A function $f(z)$ is said to belong to the class $\mathcal{L}^2(B)$ if $f(z)$ is analytic in the region B of the complex plane and is such that

(3.1.3) $$\iint_B |f(z)|^2 \, dx\, dy < \infty .$$

Let us denote by $\mathcal{E}_\rho$ the region of the complex plane enclosed by the ellipse $|z+(z^2-1)^{1/2}| = \rho, \rho > 1$. We recall from Section 0.2 of the Introduction that the remainder term, satisfies an equation of the form (equation (0.2.6)),

(3.1.4) $$R_{n+1}(f) \leq \sum_{\nu=0}^{\infty} |a_\nu|^2 \sum_{\nu=0}^{\infty} | R_{n+1}[\zeta_\nu(z,\rho)]|^2 ,$$

where the functions $\zeta_\nu(z,\rho)$, $\nu = 0, 1, 2, \ldots$, are related to the Chebyshev polynomials of the second kind. From equation (3.1.4) it may then be established that a necessary and sufficient condition for the convergence of a quadrature scheme is

(3.1.5) $$\lim_{n\to\infty} \sum_{\nu=0}^{\infty} |R_{n+1}[\zeta_\nu(z,\rho)]|^2 = 0 .$$

Using the properties of the functions $\zeta_\nu(z,\rho)$, $\nu = 0,1,2,\ldots$, Davis shows that, for quadrature formulae with $p = 1$ in equation (3.1.1), condition (3.1.5) yields a condition for the convergence of a quadrature scheme in the form

$$(3.1.6) \qquad \lim_{n \to \infty} \left(\lambda_{0,n} + \lambda_{1,n} + \cdots + \lambda_{n,n} \right)^{1/n} n^{3/2} \rho^{-n/2} = 0 \; .$$

The estimates of the coefficients $\lambda_{k,n}$, $k = 0, 1, 2, \ldots$, obtained by Ouspensky for the Newton-Cotes formulae are then used to show that condition (3.1.6) holds provided $\rho > 4$. Therefore we have Davis' result that:-

> The Newton-Cotes quadrature scheme converges when applied to a function which is analytic in the region enclosed by the ellipse $|z^2 + (z^2-1)^{1/2}| = \rho > 4$.

That the region, $\mathcal{E}_4$, is not the smallest possible region has been shown separately by Krylov [12] and Barrett [42] .

Krylov [12] , like Davis [8] , discusses the convergence of interpolatory quadrature schemes one of which is the Newton-Cotes scheme. The treatment given by Krylov is based on the convergence of the corresponding interpolation formula.

Krylov uses the expression for the remainder term in the interpolation formula in terms of a contour integral, see e.g. Szegö [17] . On examination of this contour integral it is then shown that if the function $f(z)$ is analytic in the region bounded by the curve,

$$(3.1.7) \qquad \mathcal{R}\ell \left[z \log z - (z-1) \log (z-1) \right] = 0 \, ,$$

the Newton-Cotes scheme over the interval $[0, 1]$ converges when applied to $f(x)$.

Using the same method Krylov also shows that the Gauss-Legendre quadrature scheme converges when applied to a function which is analytic on the basic interval $[-1, 1]$.

Barrett [39] on the other hand discusses the contour integral form of the remainder in the integration formula itself.

Suppose that $f(z)$ is analytic on the interval $[a, b]$. Now, from Section 2.4(b) of the previous chapter, the cut for the function $q_{n+1}(z)$ in the Newton-Cotes quadrature formula over the interval $[-1, 1]$ is $[-1, 1]$. So that from Sections 2.3 and 2.5 the remainder term in the Newton-Cotes formula is given by

(3.1.8) $$R_{n+1}(f) = \frac{1}{2\pi i} \int_C \frac{q_{n+1}(z)}{p_{n+1}(z)} f(z)\, dz$$

where

(3.1.9) $$p_{n+1}(z) = \prod_{k=0}^{n} (z - 1 + 2k/n) ,$$

(3.1.10) $$q_{n+1}(z) = \int_{-1}^{1} \frac{p_{n+1}(x)}{z - x}\, dx$$

and C is any closed contour enclosing the interval $[-1, 1]$ on and within which $f(z)$ is analytic.

Barrett's method of attack is to find asymptotic estimates of the remainder term, $R_{n+1}(f)$, given by equation (3.1.8), for large values of n . To accomplish this, useful expressions for $p_{n+1}(z)$ and $q_{n+1}(z)$ as given by equations (3.1.9) and (3.1.10) respectively are obtained. Barrett has shown [39, equation (2.1)] that

$$\log p_{n+1}(z) = \tfrac{1}{2}\log(z^2-1) + \tag{3.1.11}$$

$$+ \frac{n}{2}\left[(z+1)\log(z+1)-(z-1)\log(z-1) - 2\log 2\right] + O\left(\frac{1}{n}\right).$$

His expression for $q_{n+1}(z)$ [39, equation (3.10)] has a minor error, a factor n^{-1} is omitted and its corrected form is

$$q_{n+1}(z) = -4(2\pi)^{1/2}\left(\frac{2}{e}\right)^{n} n^{-3/2}(\log n)^{-2}\left[\frac{1}{z-1} - \frac{(-1)^n}{z+1}\right]\left[1 + o\left(\frac{1}{n}\right)\right]. \tag{3.1.12}$$

The asymptotic expressions (3.1.11.) and (3.1.12) are then substituted into equation (3.1.7). From the resulting contour integral Barrett obtains precisely the same result (with modification for the change in interval of integration) as that given by Krylov [12] .

In Section 2 of this chapter we shall discuss the convergence of the Newton-Cotes quadrature scheme using the method of Barrett of examining the contour integral form of the remainder. We shall first describe an alternative method to Barrett's for obtaining asymptotic estimates for large n of the function $q_{n+1}(z)$, given by equation (3.1.10), for two reasons.

Firstly we notice that not only are the asymptotic expressions for $q_{n+1}(z)$ and $p_{n+1}(z)$ useful for studying the convergence of the quadrature scheme but they are also useful for finding asymptotic estimates of the remainder $R_{n+1}(f)$. For this reason the expression we shall obtain for $q_{n+1}(z)$ is more realistic than Barrett's for relatively small n.

Secondly for equally spaced osculatory quadrature formulae over $[-1,1]$ the functions $\psi(z)$ and $\varphi(z)$ (equations (2.4.79) and (2.4.80)) corresponding to the functions $q_{n+1}(z)$ and $p_{n+1}(z)$ respectively are simply related to these last functions. We have

$$\varphi(z) = \left[p_{n+1}(z)\right]^2 \tag{3.1.13}$$

and

$$\psi(z) = \int_{-1}^{1} \frac{\varphi(z)\,dz}{z-x} . \tag{3.1.14}$$

Equation (3.1.11) can be used immediately to obtain an asymptotic expression for the function $\phi(z)$ given by equation (3.1.13). However Barrett's method for obtaining equation (3.1.12) does not appear suitable for finding asymptotic estimates of $\psi(z)$ given by equation (3.1.14). We can however adapt our method for $q_{n+1}(z)$ to the function $\psi(z)$.

In Section 3 we shall find asymptotic estimates for $\phi(z)$ and $\psi(z)$. These expressions are then used to show that the equally spaced osculatory quadrature scheme and the Newton-Cotes quadrature scheme have the same property with respect to convergence.

Obreschkoff type quadratures are discussed in Section 4. Krylov and Sulgina[40] have shown that the Obreschkoff quadrature scheme over $[0, 1]$ converges provided $f(z)$ is analytic in the region of the complex plane defined by

(3.1.15) $$|z(z-1)| < 1/4 .$$

We obtain this result by examining the contour integral form of the remainder.

To conclude the chapter we shall make a passing reference to the convergence of Gaussian quadrature over the interval $[-1, 1]$.

3.2 The Convergence of the Newton-Cotes Quadrature Scheme

We recall that the Newton-Cotes quadrature rule over the interval $[-1, 1]$ from Section 2.4(b) of Chapter II may be written

$$(3.2.1) \qquad \int_{-1}^{1} f(x)\,dx = \sum_{k=0}^{n} \lambda_{k,n} f(x_{k,n}) + R_{n+1}(f) .$$

The remainder term when $f(z)$ is analytic on $[-1, 1]$ from equations (3.1.8) and (2.5.1) is given by

$$(3.2.2) \qquad R_{n+1}(f) = \frac{1}{2\pi i} \int_{C} \frac{q_{n+1}(z)}{p_{n+1}(z)} f(z)\,dz$$

where the functions $q_{n+1}(z)$ and $p_{n+1}(z)$ are defined by equations (3.1.10) and (3.1.9) respectively.

In this section we shall discuss the convergence of the Newton-Cotes quadrature scheme. We shall first obtain an asymptotic expression for the function $q_{n+1}(z)$. The method of obtaining this expression we shall be able to use in the next section on osculatory quadrature. The actual estimate will be used in the following chapter, Chapter IV, in the discussion of numerical estimates of the remainder.

The proof that we shall give of the necessary and sufficient conditions for the convergence of the Newton-Cotes quadrature scheme will contain more detail than that given by Barrett.

An Alternative Derivation of the Asymptotic Form of $q_{n+1}(z)$

The polynomial $p_{n+1}(z)$ in the Newton-Cotes quadrature formula may be written

$$(3.2.3) \quad p_{n+1}(z) = \prod_{k=0}^{n} \left(z - 1 + \frac{2k}{n}\right) .$$

Following Barrett [39, equation (1.5)] we can express $p_{n+1}(z)$ in terms of Γ- functions in the form

$$(3.2.4) \quad p_{n+1}(z) = \left(\frac{2}{n}\right)^{n+1} \cdot \frac{1}{\pi} \Gamma\left[\frac{n}{2}(z+1)+1\right] \Gamma\left[-\frac{n}{2}(z-1)+1\right] \sin\left[\frac{\pi n}{2}(z-1)\right] .$$

Now since

$$(3.2.5) \quad q_{n+1}(z) = \int_{-1}^{1} \frac{p_{n+1}(x)\, dx}{z-x} ,$$

we have on substituting equation (3.2.4) into equation (3.2.5)

$$(3.2.6) \quad q_{n+1}(z) = \frac{1}{\pi}\left(\frac{2}{n}\right)^{n+1} \left\{\int_{-1}^{0} + \int_{0}^{1}\right\} \frac{\Gamma\left[\frac{n}{2}(x+1)+1\right] \Gamma\left[-\frac{n}{2}(x-1)+1\right] \sin\left[\frac{\pi n}{2}(x-1)\right]}{z-x}\, dx .$$

Replacing $\frac{n}{2}(x+1)$ by u in $-1 \leq x \leq 0$ and $-\frac{n}{2}(x-1)$ by u in $0 \leq x \leq 1$ we find that equation (3.2.6) becomes

$$(3.2.7) \quad q_{n+1}(z) = \frac{1}{\pi}\left(\frac{2}{n}\right)^{n+1} \int_0^{n/2} \left\{ \Gamma(1+u)\, \Gamma(n-u+1)\, \sin \pi u \times \right.$$
$$\left. \times \left[\frac{(-1)^n}{\frac{n}{2}(z+1)-u} - \frac{1}{\frac{n}{2}(z-1)+u} \right] \right\} du .$$

First suppose that n is even and put $2m = n$. Then equation (3.2.7) may be written

$$(3.2.8) \quad q_{n+1}(z) = \frac{1}{\pi}\left(\frac{2}{n}\right)^{n+1} \sum_{r=0}^{m-1} \int_r^{r+1} \left\{ \Gamma(1+u)\, \Gamma(n-u+1)\, \sin \pi u \times \right.$$
$$\left. \times \left[\frac{(-1)^n}{n/2(z+1)-u} - \frac{1}{\frac{n}{2}(z-1)+u} \right] \right\} du .$$

Provided z does not lie in the neighbourhood of the interval $[-1, 1]$ the sum in equation (3.2.8) is dominated by the first term. This may be shown as follows.

Let us put

$$(3.2.9) \quad U_r = \int_r^{r+1} \frac{\Gamma(1+u)\, \Gamma(n-u+1)\, \sin \pi u}{\frac{n}{2}(z+1) - u}\, du .$$

On replacing u by $u+r$ in equation (3.2.9) we have

$$(3.2.10) \quad U_r = \int_0^1 \frac{\sin \pi(u+r)\, \Gamma(1+r+u)\, \Gamma(n-u+1-r)}{\frac{n}{2}(z+1) - u - r}\, du .$$

Using the continuation formula for the Γ-function equation (3.2.10) becomes

$$(3.2.11)\quad U_r = \int_0^1 \left\{ \frac{\sin \pi u \, \Gamma(1+u)\, \Gamma(n-u+1)}{\frac{n}{2}(z+1) - u} \times \frac{(-1)^r (r+u) \ldots (1+u)}{(n-u-r) \ldots n-u} \left[1 - \frac{r}{\frac{n}{2}(z+1) - u - r} \right] \right\} du \,.$$

Summing equation (3.2.11) over r, $r = 0(1)\{m-1\}$, we have

$$(3.2.12)\quad \sum_{r=0}^{m-1} U_r = \int_0^1 \left\{ \frac{\sin \pi u \, \Gamma(1+u)\, \Gamma(n-u+1)}{\frac{n}{2}(z+1) - u} \times \left[1 - \sum_{r=1}^{m-1} \frac{(-1)^{r+1} (r+u) \ldots (1+u)}{(n-u-r) \ldots (n-u)} \left(1 - \frac{r}{\frac{n}{2}(z+1) - u - r} \right) \right] \right\} du \,.$$

The factor $1 - r/[\frac{n}{2}(z+1) - u - r]$ is $O(1)$ for all u, $0 \leq u \leq 1$, and r, $1 \leq r \leq (m-1)$, provided z does not lie in the neighbourhood of the real interval $[-1, 1]$.

Let us now consider the sum

$$(3.2.13)\quad S = \sum_{r=1}^{m-1} \frac{(-1)^{r+1} (r+u) \ldots (1+u)}{(n-u-r) \ldots (n-u)} \,.$$

The terms of S are alternating in sign and decreasing in magnitude. Therefore the value of S lies somewhere between the first, and the sum of the first two of its terms. That is

$$(3.2.14)\quad \frac{1+u}{n-u} \geqslant S \geqslant \frac{1+u}{n-u} - \frac{(1+u)(2+u)}{(n-u)(n-1+u)} \,.$$

From the inequality (3.2.14) we see immediately that S is of $O(1/n)$. Thus equation (3.2.12) becomes

$$(3.2.15)\quad \sum_{r=0}^{m-1} U_r = \int_0^1 \frac{\sin \pi u \, \Gamma(1+u)\, \Gamma[n-u+1]}{n/2(z+1) - u} \left[1 + O(\tfrac{1}{n})\right] du \; .$$

Similarly it can be shown that, provided z does not lie in a neighbourhood of the interval $[-1, 1]$,

$$(3.2.16)\quad \sum_{r=0}^{m-1} \int_r^{r+1} \frac{\Gamma(1+u)\, \Gamma(n-u+1)\, \sin \pi u}{n/2(z-1) + u} du$$

$$= \int_0^1 \frac{\sin \pi u \, \Gamma(1+u)\, \Gamma(n-u+1)}{n/2(z-1) + u} \left[1 + O(\tfrac{1}{n})\right] du \, .$$

From equations (3.2.15) and (3.2.16) we see immediately that the sum in the expression (3.2.8) for $q_{n+1}(z)$ is dominated by the first term.

A similar result is readily obtained when n is odd.

We have then, for large values of n ,

$$(3.2.17)\qquad q_{n+1}(z) \sim T_0(z)$$

where

$$(3.2.18) \qquad T_0(z) = \frac{1}{\pi}\left(\frac{2}{n}\right)^{n+1} \int_0^1 \left\{ \Gamma(1+u)\,\Gamma(n-u+1)\,\sin \pi u \times \right.$$

$$\left. \times \left[\frac{(-1)^n}{\frac{n}{2}(z+1)-u} - \frac{1}{\frac{n}{2}(z-1)+u} \right] \right\} du .$$

Since z is not too close to points of the interval $[-1, 1]$ we may replace $\frac{n}{2}(z+1) - u$ and $\frac{n}{2}(z-1) + u$ by $\frac{n}{2}(z+1)$ and $\frac{n}{2}(z-1)$ respectively in equation (3.2.18) for sufficiently large values of n.

Furthermore for $0 \le u \le 1$, $\Gamma(1+u)$ is almost constant and we shall replace it by 1. Finally if we use the fact that, see e.g. Abramowitz and Stegun [35, p.257],

$$(3.2.19) \qquad \frac{\Gamma(n+1-u)}{\Gamma(n+1)} \sim (n+1)^{-u}$$

for large n, $0 \le u \le 1$, equation (3.2.18) becomes, for large n,

$$(3.2.20) \qquad T_0(z) \doteq \frac{1}{\pi}\left(\frac{2}{n}\right)^{n+1} \Gamma(n+1) \left[\frac{(-1)^n}{\frac{n}{2}(z+1)} - \frac{1}{\frac{n}{2}(z-1)} \right] \int_0^1 n^{-u} \sin \pi u \, du .$$

Now

$$(3.2.21) \qquad \int_0^1 n^{-u} \sin \pi u \, du = \frac{1}{2i} \int_0^1 e^{-u \log n} \left[e^{i\pi u} - e^{-i\pi u} \right] du$$

$$= \frac{\pi\,(1 + 1/n)}{\pi^2 + (\log n)^2} .$$

Substituting equation (3.2.21) into equation (3.2.20) we find the required expression for $q_{n+1}(z)$ for large n,

$$(3.2.22) \qquad q_{n+1}(z) \sim -\frac{1}{n}\left(\frac{2}{n}\right)^{n+2} \frac{\Gamma(n+2)}{\pi^2+(\log n)^2}\left[\frac{1}{z-1} - \frac{(-1)^n}{z+1}\right].$$

We note at this point that if, in equation (3.2.22), we use Stirling's formula for $\Gamma(n+1)$ and neglect π^2 with respect to $(\log n)^2$ for very large n, we obtain Barrett's result, equation (3.1.12). However, for the purposes of estimating errors in Chapter IV, we shall retain the form of $q_{n+1}(z)$ given by equation (3.2.22).

<u>The Region of Convergence</u>

Let D be that region of the complex plane defined by the inequality

$$(3.2.23) \qquad Rl\left[\frac{z+1}{2}\log(z+1) - \frac{z-1}{2}\log(z-1) - \log 2\right] \leq 0$$

where $Rl(z)$ denotes the real part of the complex number z.

We shall now show that the region D has the following two properties with respect to the convergence of the Newton-Cotes quadrature scheme :

(1) if the function $f(z)$ is analytic at all points of the region D then the Newton-Cotes quadrature scheme converges when applied to $f(x)$;

(2) if $f(z)$ is not analytic at all interior points of the region D then the Newton-Cotes quadrature scheme does not converge when applied to $f(x)$.

The region D having the properties (1) and (2) above is usually referred to as the region of convergence of the Newton-Cotes quadrature scheme.

Proof of the Convergence Properties of the Region D

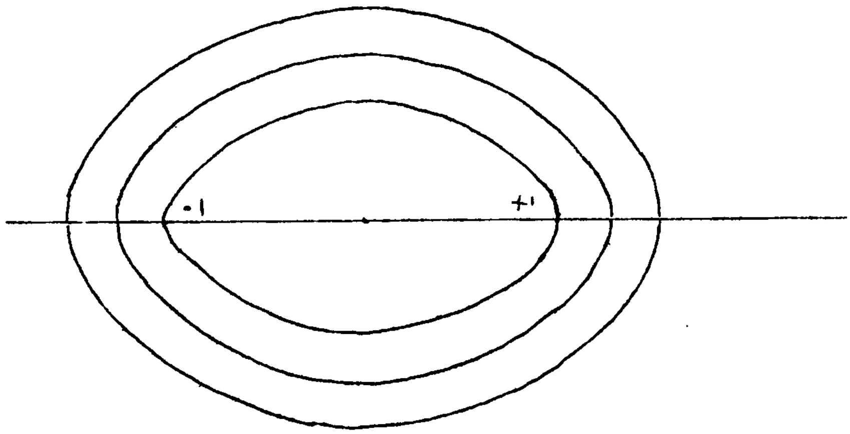
Let us denote by $\mathcal{C}_\rho$ the curve defined by

(3.2.24) $$Rl\left[\frac{z+1}{2}\log(z+1) - \frac{z-1}{2}\log(z-1) - \log 2\right] = \rho$$

where ρ is a real parameter.

The curves $\mathcal{C}_\rho$, for increasing ρ, are a set of curves symmetric about both the real and imaginary axes. We depict the curves in Fig. 3.1 below.

FIGURE 3.1



The curve $\mathcal{C}_0$ passes through the points -1 and $+1$ and forms the boundary of the region of convergence, D, defined by the inequality (3.2.23).

We now prove property (1) of the region of convergence.

Suppose $f(z)$ is analytic at all points of the region D defined by the inequality (3.2.23). Then we may take as the contour C in equation (3.2.2) one of the curves $\mathcal{C}_\rho$, $\rho > 0$. Therefore the remainder term in the Newton-Cotes integration formula is given by

$$R_{n+1}(f) = \frac{1}{2\pi i}\int_{\mathcal{C}_\rho} \frac{q_{n+1}(z)}{p_{n+1}(z)} f(z)\,dz . \tag{3.2.25}$$

Using the asymptotic expressions for $q_{n+1}(z)$ and $p_{n+1}(z)$

given by equations (3.1.12) and (3.1.11) respectively, equation (3.2.25) becomes

(3.2.26) $$R_{n+1}(f) \sim I$$

where

(3.2.27) $$I = \frac{1}{2\pi i} \cdot \frac{-4.(2\pi)^{\frac{1}{2}}}{n^{3/2}(\log n)^2} \int_{\mathcal{C}_\rho} \left[\frac{1}{z-1} - \frac{(-1)^n}{z+1}\right](z^2-1)^{-\frac{1}{2}} \times$$
$$\times \left\{\exp\left[\frac{z+1}{2}\log(z+1) - \frac{z-1}{2}\log(z-1) - \log 2\right]\right\}^{-n} f(z)\,dz.$$

Now for z on the curve $\mathcal{C}_\rho$ we can place an upper bound M, say, on that part of the integrand $f(z)(z^2-1)^{-\frac{1}{2}}\left[1/(z-1) - (-1)^n/(z+1)\right]$. Also by definition of $\mathcal{C}_\rho$ we have

(3.2.28) $$\left|\exp\left[\frac{z+1}{2}\log(z+1) - \frac{z-1}{2}\log(z-1) - \log 2\right]\right| = e^{\rho}.$$

Thus the integral on the right of equation (3.2.27) is bounded above by $M.\exp(-n\rho).\,\ell(\rho)$ where $\ell(\rho)$ is the length of the curve $\mathcal{C}_\rho$. Equation (3.2.26) now gives us

(3.2.29) $$|I| \leq \frac{4.(2\pi)^{\frac{1}{2}}}{2\pi n^{3/2}(\log n)^2} \cdot M.\,e^{-n\rho}\,\ell(\rho).$$

Since $\rho > 0$ the right hand side of the inequality (3.2.29) tends to zero as n becomes large. Hence from (3.2.26) $R_{n+1}(f)$ tends to zero as n tends to infinity.

To prove property (2) we have only to consider the remainder term when the Newton-Cotes formula is applied to the function $f(x) = 1/(x - z_0)$ where z_0 lies in D and $|Im(z_0)| > 0$.

In this case we may take as our contour C one of the curves $\mathcal{C}_\rho$ together with a small circle described in the clockwise direction about the point $z = z_0$ joined to $\mathcal{C}_\rho$ by a pair of parallel lines.

The contribution to the remainder from the parallel lines cancel. Furthermore on $\mathcal{C}_\rho$ we can place an upper bound on $1/(z - z_0)$. So that using the method in the proof of property (1) we see that the contribution to the remainder from $\mathcal{C}_\rho$ tends to zero as we let n increase.

Now from the theorem of residues the contribution from the small circle around $z = z_0$ is given by $-q_{n+1}(z_0)/p_{n+1}(z_0)$

Thus for large n we have

$$R_{n+1}(f) \sim \frac{4(2\pi)^{1/2}}{n^{3/2}(\log n)^2}\left[\frac{1}{z_0 - 1} - \frac{(-1)^n}{z_0 + 1}\right](z_0^2 - 1)^{-1/2} \times \tag{3.2.30}$$

$$\times \left\{\exp\left[\frac{z_0+1}{2}\log(z_0+1) - \frac{z_0-1}{2}\log(z_0-1) - \log 2\right]\right\}^{-n}.$$

Since z_0 lies within D the exponent of the exponential in equation (3.2.30) is negative and hence $R_{n+1}(f)$ tends to infinity with n .

We have then shown that properties (1) and (2) are satisfied by the region D defined by the inequality (3.2.23).

3.3 The Convergence of Osculatory Quadrature Formulae

In this section we shall show that D is the region of convergence of the equally spaced osculatory quadrature formula. From Section 2.4(d) the formula may be written

$$(3.3.1)\quad \int_{-1}^{1} f(x)\,dx = \sum_{k=0}^{n} \lambda_{k,0,n} f(x_{k,n}) + \sum_{k=0}^{n} \lambda_{k,1,n} f'(x_{k,n}) + R_{2n+2}(f).$$

From equation (2.5.1) the remainder term $R_{2n+2}(f)$, when $f(z)$ is analytic in the interval $[-1, 1]$, is then given by

$$(3.3.2)\quad R_{2n+2}(f) = \frac{1}{2\pi i} \int_C \frac{\psi(z)}{\varphi(z)} f(z)\,dz$$

where $\varphi(z)$ and $\psi(z)$ are defined by equations (3.1.13) and (3.1.14). The contour C is any contour which has in its interior the interval of integration $[-1, 1]$ and is such that $f(z)$ is analytic on and within C .

To investigate the behaviour of $R_{2n+2}(f)$ for large n we will first obtain asymptotic expressions for the functions $\psi(z)$ and $\phi(z)$.

Asymptotic Expressions for $\psi(z)$ and $\phi(z)$

From equations (3.1.11) and (3.1.13) the required asymptotic form of the function $\phi(z)$ is immediately obtained. We have

$$\log \phi(z) = 2 \log p_{n+1}(z) \tag{3.3.3}$$

$$= \log(z^2-1) + n\left[(z+1)\log(z+1)-(z-1)\log(z-1)-2\log 2\right] + O\left(\frac{1}{n}\right).$$

However to obtain the corresponding asymptotic expression for $\psi(z)$ is much more difficult. We follow closely the method used in Section 3.2 to find the asymptotic form of $q_{n+1}(z)$.

From equations (3.1.13) and (3.1.14) we have

$$\psi(z) = \int_{-1}^{1} \frac{[p_{n+1}(x)]^2}{z-x}\, dx. \tag{3.3.4}$$

Using the same substitutions as in Section 3.2 equation (3.3.4) becomes, for $n = 2m$,

$$(3.3.5)\qquad \psi(z) = \frac{1}{\pi^2}\left(\frac{2}{n}\right)^{2n+2}\sum_{r=0}^{m-1}\int_r^{r+1}\left[\Gamma(1+u)\,\Gamma(n-u+1)\sin\pi u\right]^2 \times$$
$$\times\left[\frac{1}{\frac{n}{2}(z+1)-u}+\frac{1}{\frac{n}{2}(z-1)+u}\right]du\,.$$

Again the major contribution to the sum, provided z does not lie too close to $[-1, 1]$ comes from the first term. To show this we follow the method of the previous section.

The sum corresponding to S in equation (3.2.13) is given by

$$(3.3.6)\qquad S_1 = \sum_{r=1}^{m-1}\frac{(r+u)^2\;.\;.\;.\;(1+u)^2}{(n-u-r)^2\;.\;.\;.\;(n-u)^2}\,.$$

The terms of S_1 are decreasing in magnitude and the first term is $O\left(\frac{1}{n^2}\right)$. Hence S_1 must be $O\left(\frac{1}{n}\right)$ which proves the required result. A similar result holds when n is odd. Therefore from equation (3.3.5) we find that, for large n,

$$(3.3.7)\qquad \psi(z) \sim T_{0,1}$$

where

$$(3.3.8)\qquad T_{0,1} = \frac{1}{\pi^2}\left(\frac{2}{n}\right)^{2n+2}\int_0^1\left[\Gamma(1+u)\;\Gamma(n-u+1)\;\sin\pi u\right]^2 \times$$
$$\times\left[\frac{1}{\frac{n}{2}(z+1)-u}+\frac{1}{\frac{n}{2}(z-1)+u}\right]du\,.$$

provided z does not lie in the neighbourhood of $[-1, 1]$.

Making the same approximations as in the case of $q_{n+1}(z)$ equation (3.3.8) takes the form

$$(3.3.9) \qquad T_{0,1} \sim \frac{[\Gamma(n+1)]^2}{\pi^2}\left(\frac{2}{n}\right)^{2n+2}\left[\frac{1}{\frac{n}{2}(z+1)} + \frac{1}{\frac{n}{2}(z-1)}\right]\int_0^1 n^{-2u}\sin^2\pi u\,du.$$

Expressing the integrand in the integral on the right of equation (3.3.9) in terms of exponentials it is readily shown that

$$(3.3.10) \qquad \int_0^1 n^{-2u}\sin^2\pi u\,du = \frac{\pi^2}{4\log n[(\log n)^2+\pi^2]}\left[1-\frac{1}{n^2}\right] .$$

Using equations (3.3.10) and (3.3.9), equation (3.3.7) gives us the asymptotic expression for $\psi(z)$,

$$(3.3.11) \quad \psi(z) \sim [\Gamma(n+1)]^2\left(\frac{2}{n}\right)^{2n+3}\frac{1}{4\log n\,[(\log n)^2+\pi^2]}\left[\frac{1}{z-1}+\frac{1}{z+1}\right].$$

<u>The Region of Convergence of Osculatory Quadrature Formulae</u>

Using Stirling's formula for $\Gamma(n+1)$ equations (3.3.11) and (3.3.3) give us

$$(3.3.12) \quad \frac{\psi(z)}{Q(z)} \sim \frac{4\pi\,(z^2-1)^{-1}}{n^2[(\log n)^2+\pi^2]}\left[\frac{1}{z+1}+\frac{1}{z-1}\right] \times$$

$$\times \left[\left\{\exp\left[\frac{z+1}{2}\log(z+1)-\frac{z-1}{2}\log(z-1)-\log 2\right]\right\}^{-2n}\right.$$

Substituting equation (3.3.12) into equation (3.3.2) we have

$$(3.3.13) \quad R_{2n+2}(f) \sim \frac{1}{2\pi i} \cdot \frac{4\pi}{n^2 \log n[(\log n)^2+\pi^2]} \int_C (z^2-1)^{-1}\left[\frac{1}{z+1}+\frac{1}{z-1}\right] \times$$

$$\times \left\{ \exp\left[\frac{z+1}{2}\log(z+1) - \frac{(z-1)}{2}\log(z-1) - \log 2\right]\right\}^{-2n} f(z)dz .$$

In proving that the region D defined by the inequality (3.2.22) is the region of convergence of the Newton-Cotes scheme the argument depended entirely on the exponent of the exponential in equation (3.2.26). We see that the exponent of exponential in equation (3.3.13) is precisely the same.

Therefore we may prove similarly that the region of convergence of the osculatory quadrature formula with equally spaced abscissae is the same as that of the Newton-Cotes quadrature scheme, i.e., the region D defined by the inequality

$$(3.3.14) \qquad Rl \left[\frac{z+1}{2}\log(z+1) - \frac{z-1}{2}\log(z-1) - \log 2\right] \leq 0 .$$

3.4 The Obreschkoff Type Quadrature Scheme

Let us consider the interval $[-1, 1]$ and suppose that the function $f(z)$ is analytic on $[-1, 1]$. Then, from Sections 2.4(e) and 2.5 of the previous chapter, the remainder term in the Obreschkoff type quadrature, equation (2.4.91) is given by

$$R_{2p}(f) = \frac{1}{2\pi i} \int_c \frac{\psi(z)}{\varphi(z)} f(z)\, dz \tag{3.4.1}$$

where C is any contour on and within which $f(z)$ is analytic and has in its interior the basic interval $[-1, 1]$.

From equations (2.4.87) and (2.4.88) the functions $\varphi(z)$ and $\psi(z)$ are given by

$$\varphi(z) = (z-1)^p (z+1)^p , \tag{3.4.2}$$

$$\psi(z) = \int_{-1}^{1} \frac{(x-1)^p (x+1)^p}{z-x}\, dx . \tag{3.4.3}$$

To investigate the convergence properties of the Obreschkoff quadrature scheme we first require asymptotic forms of these last two functions as we let p increase.

The function $\varphi(z)$ is already in a manageable form. However to find a suitable expression for $\psi(z)$ requires some analysis.

An Asymptotic Expression for $\psi(z)$ in Obreschkoff Quadrature Formulae

In finding a suitable form for $\psi(z)$ we shall make use of Laplace's method for integrals, see De Bruijn [15, Chapt.IV].

Let us write equation (3.4.3) in the form

$$\psi(z) = (-1)^p \int_{-1}^{1} g(x)\, e^{p\, h(x)}\, dx \tag{3.4.4}$$

where,

$$g(x) = \frac{1}{z-x} \tag{3.4.5}$$

and

$$h(x) = \log(1-x^2) \quad . \tag{3.4.6}$$

Now provided z is not too close to the interval $[-1, 1]$, $g(x)$ is a slowly varying function in that interval. Furthermore the function $h(x)$ has a maximum value at $x=0$; thus in the neighbourhood of $x=0$ we may approximate to $h(x)$ by $h(0) - \frac{1}{2} x^2 h''(0)$. Equation (3.4.4) now becomes

$$\psi(z) \sim (-1)^p g(0) \int_{-1}^{1} e^{p[h(0) - \frac{1}{2} x^2 h''(0)]}\, dx \quad . \tag{3.4.7}$$

For the purposes of evaluating the integral in the expression (3.4.7) we replace the interval $[-1, 1]$ by $(-\infty, \infty)$. This is permissible since it is possible to show, De Bruijn [15,p.61] that the additional contributions to the integral from the intervals $(-\infty, -1)$ and $(1, \infty)$ are negligible for large values of p.

We can now make use of the fact that, see Abramowitz and Stegun [35, p.255],

(3.4.8) $$\int_{-\infty}^{\infty} e^{-\alpha x^2}\, dx = \left(\frac{2\pi}{\alpha}\right)^{1/2}.$$

Substituting equation (3.4.8) into the expression (3.4.7) we finally obtain the required asymptotic expression for $\psi(z)$,

(3.4.9) $$\psi(z) \sim \frac{(-1)^p (2\pi)^{1/2}}{z\,|h''(0)|^{1/2}} = \frac{(-1)^p}{z}\left[\frac{\pi}{p}\right]^{1/2}.$$

The Convergence of the Obreschkoff Type Quadrature Scheme

From equations (3.4.2) and (3.4.9) we find that the asymptotic form for the ratio $\psi(z) / \varphi(z)$ is given by

(3.4.10) $$\frac{\psi(z)}{\varphi(z)} \sim \frac{(-1)^p \pi^{1/2} (z^2-1)^{-p}}{p^{1/2}}$$

for large values of p.

Substituting the expression (3.4.10) into equation (3.4.1) we have

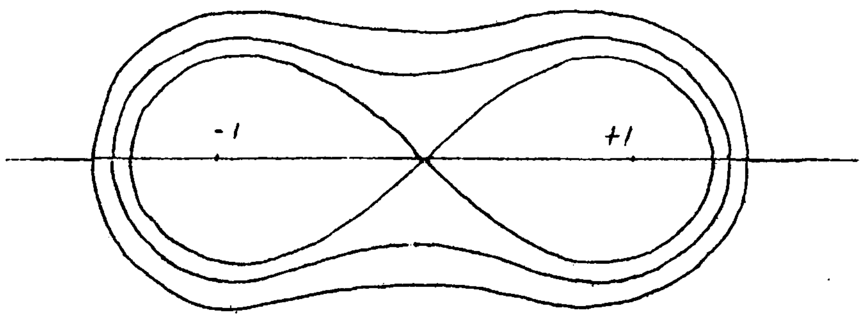
$$R_{2p}(f) = \frac{(-1)^p}{2\pi i}\left[\frac{\pi}{p}\right]^{1/2}\int_C z^{-1}(z^2-1)^{-p} f(z)\,dz. \tag{3.4.11}$$

For large p the important factor in the integral on the right of equation (3.4.11) is of course $(z^2-1)^{-p}$. Now the curves

$$|z^2-1| = \rho \tag{3.4.12}$$

where $\rho \geq 1$ is one of the Ovals of Cassini with foci at $-1, +1$, see Fig. 3.2.

FIGURE 3.2



Following the arguments used in Section 3.2 we see that the Obreschkoff type quadrature scheme has for its region of convergence the region defined by

$$|z^2 - 1| \leq 1 \quad . \tag{3.4.13}$$

This region has as its boundary the lemniscate of Bernoulli, $|z^2 - 1| = 1$.

This result but corresponding to the interval $[0, 1]$ has been given previously by Krylov and Sulgina [40] but their method of attack is somewhat different.

3.5 The Convergence of the Gauss-Jacobi Quadrature Scheme

It is well known, see Krylov [12, Chapt.12] that the Gauss-Jacobi quadrature scheme converges when applied to any function $f(z)$ which is analytic on the interval of integration $[-1, 1]$.

Suppose that $f(z)$ is analytic on the interval $[-1, 1]$. Then from equation (2.4.7) and the results of Section 2.5, mainly equation (2.5.1), the remainder term in the Gauss-Jacobi quadrature formula is given by

$$R_{n+1}(f) = \frac{1}{2\pi i} \int_C \frac{\pi_{n+1}^{(\alpha,\beta)}(z)}{P_{n+1}^{(\alpha,\beta)}(z)} f(z)\, dz \quad . \tag{3.5.1}$$

where C is any contour which surrounds $[-1, 1]$ and which does not contain any singularity of the function $f(z)$.

From Elliott and Robinson [41] the required asymptotic expression for $\Pi_{n+1}^{(\alpha,\beta)}(z) / P_{n+1}^{(\alpha,\beta)}(z)$ is given by

$$(3.5.2) \qquad \frac{\Pi_{n+1}^{(\alpha,\beta)}(z)}{P_{n+1}^{(\alpha,\beta)}(z)} \sim 2\pi (z-1)^{\alpha} (z+1)^{\beta} \left[z + (z^2-1)^{1/2} \right]^{-2n-\alpha-\beta-3}$$

for large n and z not lying in the real interval $[-1, 1]$

Now the set of curves, $\mathcal{E}_{\rho}$, defined by

$$(3.5.3) \qquad \left| z + (z^2-1)^{1/2} \right| = \rho \quad , \quad \rho \geq 1 ,$$

is a family of confocal ellipses with foci at the points ± 1
When $\rho = 1$ we have the degenerate ellipse, the real interval $[-1, 1]$.
We have already discussed this family of ellipses in the Introduction.

Now since $f(z)$ is analytic on the basic interval $[-1, 1]$ we may take the contour C to be the ellipses $\mathcal{E}_{\rho}$, $\rho > 1$.
Using the expression (3.5.2) and equation (3.5.1) we then have

$$(3.5.4) \qquad R_{n+1}(f) \sim \frac{1}{2\pi i} \int_{\mathcal{E}_{\rho}} \frac{2\pi (z-1)^{\alpha} (z+1)^{\beta}}{\left[z + (z^2-1)^{1/2} \right]^{2n+\alpha+\beta+3}} f(z) \, dz .$$

Again using the methods described in the previous sections of this chapter it is easily shown that the region of convergence of the Gauss-Jacobi quadrature scheme is given by

$$|Z + (Z^2 - 1)^{1/2}| \leq 1 \tag{3.5.5}$$

which is simply the interval $[-1, 1]$.

Summary

In this chapter we have considered the question of the convergence of several well known quadrature schemes when these schemes were applied to analytic functions.

With a finite interval $[a, b]$ and under the assumption that the function $f(z)$ has no singularities in the interval of integration the remainder term was expressed in terms of an integral around a closed contour which had the basic interval $[a, b]$ in its interior. An asymptotic expression for this remainder was obtained. On examination of this expression the regions of convergence for several quadrature rules were found.

CHAPTER IV

ASYMPTOTIC ESTIMATES OF THE REMAINDER TERM

4.1 Introduction

In Chapter I we obtained an expression in the required form of a contour integral for the remainder term $R_{n+1}(f)$ in a general quadrature formula. We shall now make use of this expression to find estimates of the remainder for large values of n. As we have indicated in the introduction it is often found that methods which are used for large values of n yield realistic results even for small n.

We shall consider almost exclusively those formulae satisfying the conditions of Theorem 1. Our starting point is then the contour integral expression given by equation (1.2.2) in the form

(4.1.1) $$R_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\}\frac{\psi(z)}{\varphi(z)}\, f(z)\, dz$$

where the contours C^+ and C^- satisfy the conditions of Theorem 1.

The contours C^+ and C^- may be deformed in any way provided that the deformation accords with the conditions of the Theorem. Any possible deformation near the end points of the interval has been discussed at some length in Chapter II and we will frequently refer to the results obtained in that Chapter.

We recall that the contours C^+ and C^- lie in the region D_1 of the complex plane in which the function $f(z)$ is analytic. We find that the final choice of the contours depends to a great extent on the nature of the singularities of the function $f(z)$. The functions which we shall consider here fall into one of the following categories:

(a) functions whose only singularities in the finite part of the complex plane are poles;

(b) functions which have branch points at the end points of the interval of integration; the methods are readily applicable to functions with branch points outside the interval of integration and we shall consider the case of a branch point on the real axis in the discussion of the Gauss-Jacobi quadrature formulae;

(c) entire functions, i.e., functions with no singularities in the finite part of the complex plane;

(d) functions which have an essential singularity at an end point of the interval $[a, b]$.

Once we have established the general form of the contours C^+ and C^- we can make use of known asymptotic expressions for the ratio $\psi(z)/\varphi(z)$ for large values of n . The reason for introducing the asymptotic expressions is simply that these expressions for the ratio $\psi(z)/\varphi(z)$, usually defined in terms of higher transcendental functions, are given in terms of elementary functions. The resulting contour integral should then be easier to manipulate.

Suppose in the first instance that the contours C^+ and C^- lie in some region of the complex plane in which the asymptotic expression

$$(4.1.2) \qquad \frac{\psi(z)}{\varphi(z)} \sim K(z),$$

for large values of n , is valid. Then, from the expression (4.1.2) and equation (4.1.1) our main task is the evaluation of the integral,

$$(4.1.3) \qquad E_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} K(z) f(z)\, dz \quad .$$

The approximate evaluation of the contour integral in equation (4.1.3) will then give us estimates of the remainder term $R_{n+1}(f)$ for large n .

This Chapter is divided into several Sections. In Section 4.2 we shall describe a general approach to the problem while in the succeeding Sections we shall deal exclusively with particular quadrature formulae. We shall consider, in turn, the Gauss-Jacobi, Gauss-Laguerre, Gauss-Hermite and the Newton-Cotes formulae. In the final Section we shall consider the extension of these results to other quadrature rules.

4.2 A General Approach

In this Section we shall consider the application of the integration formula, given by equation (0.1.2), to functions of the types (a), (b), (c) and (d) mentioned in the previous Section, Section 4.1. For each type of function we shall describe a general approach to the problem of finding estimates of the remainder term $R_{n+1}(f)$ given by equation (4.2.1)

Our first concern is the deformation of the contours C^+ and C^-.

To simplify this discussion let us choose a family of contours Γ_ρ, with parameter $\rho \geq 0$, which has the following properties:

(1) if ζ is a point on the curve Γ_ρ then $|\zeta|$ tends to infinity as we let ρ tend to infinity;

(2) there is a lower limit, ρ_0 (say), of the parameter ρ such that the interval of integration (with the exception of the point at infinity when the interval of integration is infinite) just remains within or is part of the curve Γ_{ρ_0}

The family of curves is usually suggested by the function $K(z)$ on the right of the asymptotic expression (4.1.2). We expect to be able to write for ζ on Γ_ρ

$$(4.2.1) \qquad |K(z)| = |g(\zeta)| \cdot F(\rho)$$

where $F(\rho)$ is a constant on Γ_ρ.

We have already discussed a few such families of curves in Chapter III. As a particular example let us consider the Gauss-Legendre quadrature formula. In this case it is found that

$$K(z) = \frac{2\pi}{\{z + (z^2-1)^{1/2}\}^{2n+3}}$$

Now $|z + (z^2-1)^{1/2}| = \rho\ (\geqslant 1)$ is an ellipse, $\mathcal{E}_\rho$, with foci at ± 1. We would therefore take as our family of contours for Gauss-Legendre quadrature the family of ellipses $\mathcal{E}_\rho$.

We shall further simplify the general discussion by choosing the functions $\psi(z)$ and $\varphi(z)$ to satisfy the conditions of Corollary 1 and suppose that the interval of integration and the cut for the function $\psi(z)$ coincide. Therefore the ratio $\psi(z)/\varphi(z)$ has no singularities in the complex plane cut along $[a, b]$.

Let us now consider the remainder term according to the type of function

4.2(a) When $f(z)$ is a Meromorphic Function of z.

Suppose $f(z)$ has a simple pole at the point $z = z_0$ where the imaginary part of z_0 $(\operatorname{Im}(z_0)) > 0$. Suppose also that there are no other singularities of $f(z)$ in the finite complex plane. Then we may write

$$(4.2.2) \qquad f(z) = \frac{f_1(z)}{z - z_0}$$

where $f_1(z)$ is analytic in the finite complex plane.

In this case we choose our contour C^+ to consist of the following simple contour, see Fig. 4.1,

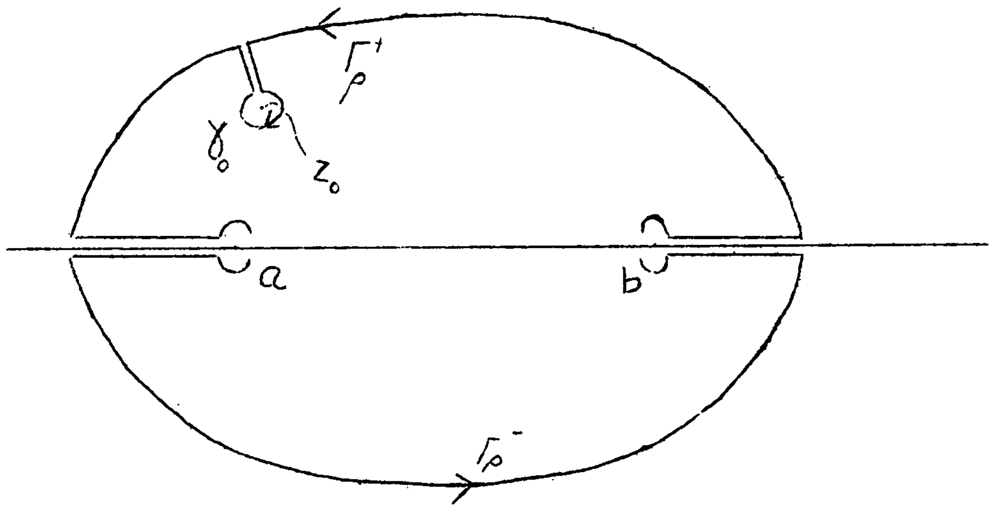
(1) semi-circular indentations at the end points a and b;

(2) that part, Γ_ρ^+, lying in the upper half-plane of one of the family of curves Γ_ρ, $\rho > \rho_0$, described in a counterclockwise direction; the parameter ρ is chosen large enough so that the point z_0 lies within Γ_ρ;

(3) a small circle γ_c around the point $z = z_0$ described in a clockwise direction;

(4) the semi-circular indentations at a and b are joined to Γ_ρ^+ by lines along the upper edges of the x-axis, while γ_0 is joined to Γ_ρ^+ by a pair of parallel lines.

FIGURE 4.1



The contour C^- consists of that part of Γ_ρ lying in the lower half-plane joined to semi-circular indentations below the points a and b along the lower edge of the real axis.

The contribution to the remainder from the various parts of C^+ and C^- is as follows.

The function $f(z)$ does not have singularities at the end points of the range of integration. Thus from the results of Chapter II, Section 2.3(a), the contributions from the semi-circular indentations at a and b will either tend to zero with the radius of the semi-circles or contribute, when the end point is an abscissa, to the quadrature sum.

It may be possible to show that the contribution to the integrand from Γ_ρ tends to zero as we let ρ tend to infinity. If not, we would use one of the methods which we shall outline in Section 4.2(c) to estimate the contribution from Γ_ρ.

The contributions from the parallel lines joining Γ_ρ to γ_0 cancel and, in this case, so do the contributions from the lines parallel to the x-axis joining a to Γ_ρ and b to Γ_ρ.

Finally using equations (4.2.2) and (4.1.1) we find from the theory of residues that the contributions from the small circle γ_0, $R_{n+1}(f, \gamma_0)$, is given by

$$R_{n+1}(f, \gamma_0) = -\frac{\psi(z_0)}{\varphi(z_0)} \cdot f_1(z_0) \tag{4.2.3}$$

For large n it is more convenient to use the asymptotic expression for $\psi(z)/\varphi(z)$ given by equation (4.1.2). We have $R_{n+1}(f, \gamma_0) \sim E_{n+1}(f, \gamma_0)$ where,

$$(4.2.4) \qquad E_{n+1}(f, \gamma_0) = -K(z_0)\, f_1(z_0)\,.$$

In many cases it is found that equation (4.2.4) provides the major contribution to the remainder term $R_{n+1}(f)$.

For a function with several simple poles at the points $z = z_r,\ r = 1(1)m$, we find immediately that the contribution from the circles $\gamma_r,\ r = 1(1)m$, surrounding the poles is given by

$$(4.2.5) \qquad \sum_{r=1}^{m} E_{n+1}(f, \gamma_r) = -\sum_{r=1}^{m} K(z_r)\, f_r$$

where f_r is the residue of $f(z)$ at the point $z = z_r$.

A Pole of Order p

Suppose $f(z)$ has a pole of order p at $z = z_0$. Then the contribution from the integral around the circle γ_0 is given by (compare equation (1.3.15))

$$(4.2.6) \qquad E_{n+1}(f, \gamma_0) = -\frac{1}{(p-1)!}\,\frac{d^{p-1}}{dz^{p-1}}\left[(z-z_0)^p K(z) f(z)\right]$$

evaluated at $z = z_0$.

<u>Notes</u>: We have assumed above that the function $\psi(z)/\phi(z)$ has no singularities in the complex plane cut along $[a, b]$. Modifications must of course be made when this is not so. There are two important cases:

(i) when the cut for the function $\psi(z)$ extends beyond the interval $[a, b]$ the contribution from the lines parallel to the x-axis joining the end points to the curve Γ_ρ will not cancel;

(ii) when $\phi(z)$ has a zero at the point $z = \zeta$ (say), outside the interval $[a, b]$ we must treat the point as we treated any pole of the function $f(z)$.

These notes also apply to the following cases.

4.2(b) When $f(z)$ has a Branch Point at $z = a$.

Suppose that the function $f(z)$ has a branch point at the end point a of the interval of integration $[a, b]$ and that this is the only singularity of $f(z)$ in the finite part of the complex plane. Then we shall cut the plane from a to $-\infty$ along the negative direction of the real axis. Thus if ζ is a point on the real axis such that $-\infty < \zeta < a$ we have

(4.2.7) $$f(\zeta + i0) \neq f(\zeta - i0) .$$

The contours C^+ and C^- are those depicted in Fig. 4.1 except for the parallel lines and the small circle associated with the point z_0.

Now the contributions from the semi-circular indentations at both a and b have been considered in Sections 2.3(b) and 2.3(a) respectively and the contributions from the parallel lines joining b to Γ_ρ cancel. Furthermore it may be possible to show that the contributions from the integral along Γ_ρ tends to zero as ρ tends to infinity; if not we would use Section 4.2(c) below to estimate this contribution.

Most important in this case is the contribution from the parallel lines joining the point a to the curve Γ_ρ. Suppose that Γ_ρ meets the real axis at the point a' where $a' < a$ and let us denote by $R_{n+1}(f, a'a)$ the contribution to the remainder term from these parallel lines. We thus have from equation (4.1.1)

$$(4.2.8)\quad \begin{cases} R_{n+1}(f, a'a) = \dfrac{1}{2\pi i}\displaystyle\int_{a'}^{a} \dfrac{\psi(x)}{\varphi(x)} f(x+oi) + \dfrac{1}{2\pi i}\displaystyle\int_{a}^{a'} \dfrac{\psi(x)}{\varphi(x)} f(x-oi)\,dx \\[2ex] \qquad = \dfrac{1}{2\pi i}\displaystyle\int_{a'}^{a} \dfrac{\psi(x)}{\varphi(x)} \left[f(x+oi) - f(x-oi)\right] dx \end{cases}$$

In the cases we have considered the asymptotic form which is used for points on the curve $\Gamma_\rho,\ \rho > \rho_0$, is not valid in the neighbourhood of the end point a . An alternative asymptotic expression which is valid at the point a must therefore be found.

Suppose then that $\psi(z)/\varphi(z) \sim K_1(z)$ in a region of the complex plane which includes the interval $(-\infty, a]$. Further, suppose that the contribution to the curve Γ_ρ tends to zero as we let ρ tend to infinity. Then from equation (4.2.8) we have $R_{n+1}(f) \sim E_{n+1}(f)$ where

$$E_{n+1}(f) = \frac{1}{2\pi i} \int_{-\infty}^{a} K_1(x) \left[f(x+0i) - f(x-0i) \right] dx \ . \tag{4.2.9}$$

The problem is then reduced to finding an estimate of the real integral on the right of equation (4.2.9) for large values of n . Considerable ingenuity is needed but Laplace's method for integrals, see De Bruijn [15, Chapt. IV] , appears to provide a standard attack to the problem.

4.2(c) Entire Functions

When the function $f(z)$ has no singularities in the finite part of the complex plane there are two possible approaches.

Firstly we attempt to minimise the modulus of the remainder term over a given set of curves. Davis and Rabinowitz [9] have used this technique with respect to the set of areas contained within the ellipses $\mathcal{E}_\rho$, see Section 0.2. Secondly it may be possible to use the saddle point method, see De Bruijn [15, Chapt. V] . In either case our starting point is the contour integral form of the remainder term given by equation (4.1.1).

(i) Bounds for $|E_{n+1}(f)|$

Let us suppose that the interval $[a, b]$ is finite and that $\psi(z)/\varphi(z)$ has no singularities in the complex plane cut along $[a, b]$. Then since $f(z)$ has no singularities on $[a, b]$ the remainder term from equation (2.5.1) is given by

$$R_{n+1}(f) = \frac{1}{2\pi i} \int_C \frac{\psi(z)}{\varphi(z)} f(z)\, dz \qquad (4.2.10)$$

where C is any closed contour which has the interval $[a, b]$ in its interior. Using the asymptotic expression (4.1.2) we see that $R_{n+1}(f) \sim E_{n+1}(f)$ where

$$E_{n+1}(f) = \frac{1}{2\pi i} \int_C K(z)\, f(z)\, dz \;. \qquad (4.2.11)$$

Now let us suppose that for points z on the curve Γ_ρ we can write, see equation (4.2.1), (4.2.12) $$K(z) = |g(z)| \cdot F(\rho)$$

and that,

(4.2.13) $$G(\rho) = \max_{z \in \Gamma_\rho} |g(z)| \, .$$

Also since $f(z)$ is an entire function of z we can place an upper bound, $M(\rho)$ (say), on $|f(z)|$ for z on Γ_ρ .

Let us now take the contour C in equation (4.2.11) to be the curve Γ_ρ . Using Schwarz's inequality in conjunction with equations (4.2.12) and (4.2.13), equation (4.2.11) gives us

(4.2.14) $$|E_{n+1}(f)| \leq \frac{1}{2\pi} G(\rho) \, . \, F(\rho) \, . \, \ell(\rho) \, . \, M(\rho)$$

where $\ell(\rho)$ is the length of the curve Γ_ρ .

Now for each ρ the quantity $\mathcal{F}(\rho)$ defined by

(4.2.15) $$\mathcal{F}(\rho) = \frac{1}{2\pi} G(\rho) \, . \, F(\rho) \, . \, \ell(\rho)$$

depends only on the quadrature rule. It need, therefore, be computed only once for all functions $f(z)$.

We expect that as ρ increases $\mathcal{F}(\rho)$ will decrease while $M(\rho)$ will increase; if $[a, b]$ includes the origin then by the

Maximum Modulus theorem $M(\rho)$ certainly does increase. The most suitable choice of ρ will be that value which makes the product $\mathcal{F}(\rho).\ M(\rho)$ a minimum.

It is of interest at this point to recall the work of Davis and Rabinowitz [9] . From equations (0.2.6), (0.2.7) and (0.2.9) of the Introduction we have the inequality

(4.2.15A) $$R_{n+1}(f) \leq \sigma_\rho (\pi a b)^{1/2} .\ M(\rho).$$

The quantities a and b are the semi-major and semi-minor axes of the ellipse $\mathcal{E}_\rho$ and $M(\rho)$ is the maximum value of $|f(z)|$ in the region containing the ellipse and its interior.

The inequality (4.2.15A) may then be compared directly with the inequality (4.2.14). Numerical comparisons are made in Tables 4.3.3 and 4.6.3.

This method does not appear to be applicable to integration formulae in which the interval of integration is not finite. The saddle point method which we shall now describe should, however, be useful for such formulae.

(ii) The Saddle Point Method

Our starting point is once more the contour integral form of the remainder term given by equation (4.1.1) and since we are examining this contour integral for large n the saddle point method suggests itself quite naturally.

Let us suppose that the integrand on the right of equation (4.1.1) has clearly defined saddle points. Then we shall deform the contours C^+ and C^- to pass through these saddle points in the direction of the line of steepest descent. Our main concern in this section is the contribution to the remainder term from those parts of the contours in the neighbourhood of the saddle points.

Again it is usually more convenient to examine the quantity $E_{n+1}(f)$ given by equation (4.1.3) in the form

(4.2.16) $$E_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} K(z)\, f(z)\, dz .$$

Let us write the integrand in equation (4.2.16) in the form

(4.2.17) $$K(z)\, f(z) = h(z) \exp[\chi(z)]$$

where $h(z)$ is a slowly varying function of z in the neighbourhood of a saddle point. From equation (4.2.17) the saddle points are the solutions of the equation

(4.2.18) $$\chi'(z) = 0 .$$

It can be shown that the contribution to $E_{n+1}(f)$ from that part of the contour in the neighbourhood of the saddle point, $z = \zeta$, is asymptotically equal to (see De Bruijn [15, Chapt. V])

(4.2.19) $$\frac{1}{2\pi i} \cdot (2\pi)^{1/2} \alpha |\chi''(\zeta)|^{-1/2} \cdot h(\zeta) \cdot \exp[\chi(\zeta)] .$$

where α is a unit vector along the line of steepest descent and is given by

(4.2.20) $$|\alpha| = 1 \quad , \quad \arg\alpha = \tfrac{1}{2}\pi - \tfrac{1}{2}\arg[\chi''(\zeta)] .$$

In general it will not be possible to solve equation (4.2.18) exactly but an approximate location of the saddle point is usually sufficient.

The process can of course be generalised to the consideration of more than one saddle point.

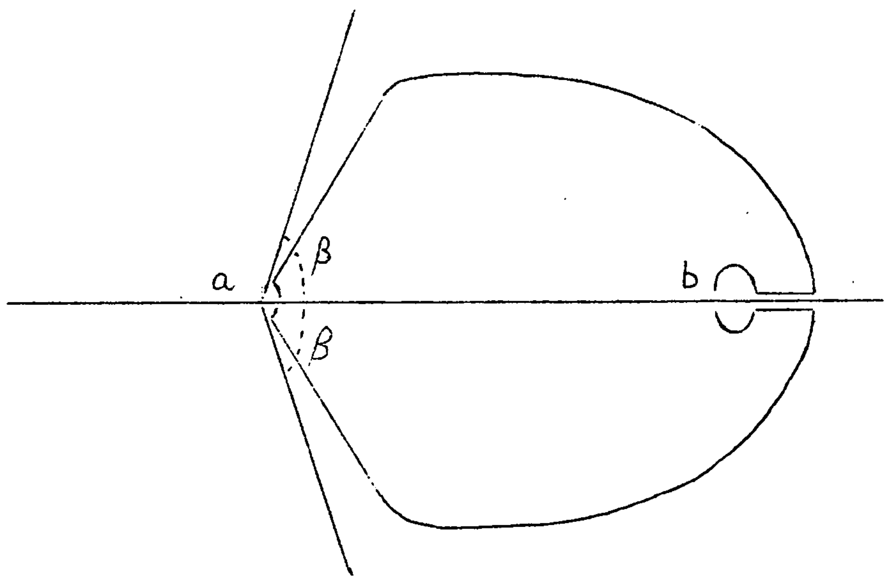
When the interval of integration is infinite it appears, see Section 4.4(c), that this is the only method applicable.

4.2(d) When $f(z)$ has an Essential Singularity at the End Point a

Let us suppose that $f(z)$ has an essential singularity at the end point a and that $f(z)$ has no other singularities in the finite complex plane.

We can take the contours C^+ and C^- at the end point b to be that depicted in Fig. 4.1. However at the end point a we take, instead of semi-circular arcs, arcs of angle less than β above and below a (see Section 2.4(c)). The contour Γ_ρ is then deformed so that it will approach the point a within the sector $|\arg(z-a)| < \beta$, see Fig. 4.2.

FIGURE 4.2



The contributions from the arcs above and below both a and b have been considered in Section 2.3. Also the contribution from the parallel lines joining b to Γ_ρ cancel.

To estimate the contribution from the remaining parts of the contours C^+ and C^- we use the saddle point method described in Section 2.4(c) above.

This concludes the general discussion. We shall now look at some explicit quadrature rules and functions.

4.3 Gauss-Jacobi Quadrature Formulae

In Section 2.4 of Chapter II an expression for the remainder term in the Gauss-Jacobi quadrature formula was obtained. From equation (2.4.7) we have

$$R_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} \frac{\Pi_{n+1}^{(\alpha,\beta)}(z)}{P_{n+1}^{(\alpha,\beta)}(z)} \cdot f(z)\, dz \tag{4.3.1}$$

where $P_{n+1}^{(\alpha,\beta)}(z)$ is the Jacobi polynomial of degree $(n+1)$ and $\Pi_{n+1}^{(\alpha,\beta)}(z)$ is given by equation (2.4.5).

The functions $\Pi_{n+1}^{(\alpha,\beta)}(z)$ and $P_{n+1}^{(\alpha,\beta)}(z)$ satisfy the conditions of Corollary 1, and the cut for the function $\Pi_{n+1}^{(\alpha,\beta)}(z)$ is the interval of integration $[-1,1]$. Furthermore all the zeros of $P_{n+1}^{(\alpha,\beta)}(z)$ lie in the interior of $[-1,1]$. Therefore the function $\Pi_{n+1}^{(\alpha,\beta)}(z) / P_{n+1}^{(\alpha,\beta)}(z)$ has no singularities in the complex plane cut along $[-1,1]$.

The general method described in the previous section, Section 4.2, may then be applied immediately.

Suitable asymptotic expressions for the functions $P_{n+1}^{(\alpha,\beta)}(z)$ and $\Pi_{n+1}^{(\alpha,\beta)}(z)$ have been obtained by Elliott and Robinson [41] and [42]. For any region of the complex plane which excludes a neighbourhood of the interval $[-1, 1]$ we have [41, equations (3.13) and (3.12)] for large n,

(4.3.2) $$\Pi_{n+1}^{(\alpha,\beta)}(z) \sim \left(\frac{\pi}{n+1}\right)^{1/2} \frac{2^{\frac{\alpha+\beta+1}{2}}(z-1)^{\alpha/2-1/4}(z+1)^{\beta/2-1/4}}{\left[z+(z^2-1)^{1/2}\right]^{\frac{2n+\alpha+\beta+3}{2}}}$$

and

(4.3.3) $$P_{n+1}^{(\alpha,\beta)}(z) \sim \frac{1}{[2\pi(n+1)]^{1/2}} \frac{2^{\frac{\alpha+\beta}{2}}\left[z+(z^2-1)^{1/2}\right]^{\frac{2n+\alpha+\beta+3}{2}}}{(z-1)^{\alpha/2-1/4}(z+1)^{\beta/2+1/4}}.$$

In these last two expressions the branches of $(z+1)^{\alpha}$ and $(z-1)^{\beta}$ are specified by the requirements $|\arg(z+1)| < \pi$ and $|\arg(z-1)| < \pi$ respectively.

From equation (4.3.2) and (4.3.3) we obtain an asymptotic form for the function $K(z)$ which is valid in any region of the complex plane excluding a neighbourhood of $[-1, 1]$. We have

(4.3.4) $$K(z) = \frac{2\pi(z-1)^{\alpha}(z+1)^{\beta}}{\left[z+(z^2-1)^{1/2}\right]^{2n+\alpha+\beta+3}}.$$

Equation (4.3.4) is the form used by Barrett [19] in his investigation of the convergence properties of the Gauss-Jacobi quadrature formulae.

The factor $Z + (Z^2-1)^{1/2}$ occurs on the right of equation (4.3.4). As we have pointed out before $|Z+(Z^2-1)^{1/2}| = \rho\ (\geq 1)$ is one of a family of ellipses with foci at ± 1. The major axis has length $\frac{1}{2}(\rho + 1/\rho)$ and the minor $\frac{1}{2}(\rho - 1/\rho)$.

Equation (4.3.4) suggests then that we should take as our family of curves, Γ_ρ, for the Gauss-Jacobi quadrature formulae, the family of ellipses, $\mathcal{E}_\rho$, defined by $|Z+(Z^2-1)^{1/2}| = \rho(\geq 1)$. Corresponding to equation (4.2.1) we have for ζ on $\mathcal{E}_\rho$

$$(4.3.5) \qquad K(\zeta) = |g(\zeta)|\ \rho^{-(2n+\alpha+\beta+3)}$$

where

$$(4.3.6) \qquad g(\zeta) = 2\pi(\zeta-1)^{\alpha}(\zeta+1)^{\beta}.$$

4.3(a) When $f(Z)$ is a Meromorphic Function of Z

Suppose $f(Z)$ has a simple pole at the point $Z = Z_0$ and that this is the only singularity of $f(Z)$ in the finite part of the complex plane. Then we may take the contours C^+ and C^- to be those depicted in Fig. 4.1 with the large contour Γ_ρ taking the form of the ellipse $\mathcal{E}_\rho$.

Following Section 4.2(a) the contribution from the parallel lines from -1 and $+1$ to $\mathcal{E}_\rho$ cancel. Also since the end points -1 and $+1$ are not abscissae of the quadrature rule the contribution from the arcs above and below a and b tend to zero with the radii of the arcs.

If we can show that the integral around the ellipse $\mathcal{E}_\rho$ tends to zero as we let ρ increase then the remainder term will be given by the integral around the small circle γ_0. Substituting equation (4.3.4) into equation (4.2.4) we find

(4.3.7) $$E_{n+1}(f) = -\frac{2\pi (z_0-1)^\alpha (z_0+1)^\beta}{\left[z_0 + (z_0^2-1)^{\frac{1}{2}}\right]^{2n+\alpha+\beta+3}} \, f_1(z_0)$$

where $f_1(z_0)$ is the residue of $f(z)$ at $z = z_0$.

The process is immediately generalised to a consideration of more than one simple pole.

Example: Let us consider the numerical integration of the function $f(z)$ defined by

(4.3.8) $$f(z) = \frac{k}{(k^2+1) - (k^2-1)\cos \pi z}$$

over the interval $[-1, 1]$ using the Gauss-Legendre quadrature formula.

Now $f(z)$ has simple poles at the points z_m given by

$$z_m = 2m \pm \frac{i}{\pi} \operatorname{arcosh}\left[\frac{k^2+1}{k^2-1}\right], \quad m = 0, \pm 1, \pm 2, \ldots \tag{4.3.9}$$

The residue of $f(z)$ at $z = z_m$ is $-i/2\pi$ when $Im(z) > 0$, and $+ i/2\pi$ when $Im(z) < 0$.

We have then an infinity of poles lying on the lines $y = \pm \pi^{-1} \operatorname{arcosh}[(k^2+1)/(k^2-1)]$. The parameter ρ is chosen such that the ellipse $\mathcal{E}_\rho$ does not pass through any of the poles of $f(z)$; on such an ellipse we may thus place an upper bound M (say), on $f(z)$. To show that the contribution $E_{n+1}(f, \mathcal{E}_\rho)$ to $E_{n+1}(f)$ from the integral along $\mathcal{E}_\rho$ tends to zero as we let ρ increase, we proceed as follows.

We have to consider the integral

$$E_{n+1}(f, \mathcal{E}_\rho) = \frac{1}{2\pi i} \int_{\mathcal{E}_\rho} \frac{2\pi f(z)}{\rho^{(2n+3)}} \, dz \; . \tag{4.3.9A}$$

Now the length of the ellipse $\mathcal{E}_\rho$ is certainly less than that of a circle of radius $\frac{1}{2}(\rho + 1/\rho)$. Using Schwarz's inequality equation (4.3.9A) then gives us

$$|E_{n+1}(f, \mathcal{E}_\rho)| \leq \frac{\pi(\rho + 1/\rho) \cdot M}{\rho^{2n+3}} \; . \tag{4.3.10}$$

Letting ρ increase indefinitely we see immediately that $|E_{n+1}(f, \mathcal{E}_\rho)|$ tends to zero. It should be stressed that we let ρ increase in such a way that $\mathcal{E}_\rho$ does not pass through a pole of $f(z)$.

It is now easy to show that the major contribution to $E_{n+1}(f)$ comes from the pair of poles at $z = \pm\frac{i}{\pi}\operatorname{arcosh}[(k^2+1)/(k^2-1)]$. Thus from equation (4.3.7) we have approximately

$$E_{n+1}(f) = \frac{2(-1)^{n+1}}{\left[S + (S^2-1)^{1/2}\right]^{2n+3}} \tag{4.3.11}$$

where $S = \pi^{-1}\operatorname{arcosh}[(k^2+1)/(k^2-1)]$. We compare the estimates of the remainder term with the actual remainder in Table 4.3.1.

TABLE 4.3.1

Actual and Estimated values of the remainder in the numerical integration of $\int_{-1}^{1}\{k/[(k^2+1)-(k^2-1)\cos\pi x]\}\,dx = 1.0 \;(k=1.2)$ using Gauss-Legendre Quadrature

n	Actual $R_{n+1}(f)$	Estimated $R_{n+1}(f)$
2	-0.0139	-0.0146
4	-0.000846	-0.000881
6	-0.0000510	-0.0000530
8	-0.00000307	-0.00000319
10	-0.00000018	-0.00000019

4.3(b) When $f(z)$ has an algebraic singularity at $z=-1$

Suppose $f(z)$ has a branch point at -1 and that $f(z)$ has no other singularities in the finite complex plane. We may then follow Section 4.2(b).

From Sections 2.3(a) and 2.3(b) of Chapter II we see that the contribution from the semi-circles above and below the end points ± 1 tend to zero as we let the radii of the semi-circles tend to zero. Furthermore the contributions from the parallel lines joining b to $\mathcal{E}_\rho$ cancel.

Let us also suppose that the integral around the ellipse $\mathcal{E}_\rho$ tends to zero as we let ρ become large.

Therefore if $K_1(z)$ is an asymptotic expression for $\pi\Pi_{n+1}^{(\alpha,\beta)}(z)/P_{n+1}^{(\alpha,\beta)}(z)$ which is valid for z in the real interval $(-\infty,-1)$ equation (4.2.8) gives us

$$E_{n+1}(f) = \frac{1}{2\pi i}\int_{-\infty}^{-1} K_1(x)\left[f(x+0i)-f(x-0i)\right]dx \qquad (4.3.12)$$

Unfortunately the asymptotic expression given by equation (4.3.4) is not valid near -1. However from Elliott and Robinson [42] we have the following asymptotic expressions which are valid in the whole open interval $(-\infty,-1)$. From [42, equations (1.17) and (1.18)] we obtain

$$(4.3.13)\qquad P_{n+1}^{(\alpha,\beta)}(z) \sim \frac{(-1)^{n+1}\, 2^{\frac{\alpha+\beta+1}{2}}\, \xi^{1/2}}{(-z-1)^{\beta/2+1/4}(-z+1)^{\alpha/2+1/4}} \cdot I_\beta(2k\xi)$$

and

$$(4.3.14)\qquad \Pi_{n+1}^{(\alpha,\beta)}(z) \sim \frac{(-1)^{n}\, 2^{\frac{\alpha+\beta+3}{2}}\, \xi^{1/2}}{(-z-1)^{-\beta/2+1/4}(-z+1)^{\alpha/2+1/4}} K_\beta(2k\xi)$$

where $z = -\cosh 2\xi$, $k = n+1+\frac{\alpha+\beta+1}{2}$ and $I_\beta(z)$ and $K_\beta(z)$ are modified Bessel functions.

Using equations (4.3.13) and (4.3.14) the required expression for $K_1(z)$ is given by

$$(4.3.15)\qquad K_1(z) = -2\,(-z-1)^{\beta}(-z+1)^{\alpha}\, \frac{K_\beta(2k\xi)}{I_\beta(2k\xi)} .$$

Substituting equation (4.3.15) into equation (4.3.12) and putting $-x = \cosh\theta$ we find

$$(4.3.16)\qquad E_{n+1}(f) = -\frac{1}{\pi i}\int_0^\infty \left[f(-\cosh\theta+0i) - f(-\cosh\theta-0i)\right]\sinh\theta \,\times$$
$$\times\,(\cosh\theta-1)^{\beta}(\cosh\theta+1)^{\alpha}\,\frac{K_\beta(k\theta)}{I_\beta(k\theta)}\, d\theta .$$

Now for large value of n , and hence k ,

$$(4.3.17)\qquad \frac{K_\beta(k\theta)}{I_\beta(k\theta)} \sim \pi e^{-2k\theta} .$$

This suggests the estimation of the integral on the right of equation (4.3.16) by Laplace's method for integrals. It also suggests that the major contribution may come from those values of θ close to zero.

We shall now illustrate how we may be able to estimate $E_{n+1}(f)$ from equation (4.3.16), by means of an example.

Example: Consider the function $f(x) = (x+1)^{\varphi}$, $0 < \varphi < 1$. (We cannot in this case estimate the remainder term from an expression in terms of derivatives because the derivatives of $f(x)$ are undefined at $x = -1$.)

We have

$$(4.3.18) \qquad f(x+0i) - f(x-0i) = 2i \sin \pi\varphi (x+1)^{\varphi}, \quad -\infty < x < 1.$$

It is readily seen that the integral around $\mathscr{E}_{\rho}$ tends to zero as we let ρ tend to infinity.

Therefore substituting equation (4.3.18) into equation (4.3.16) we have

$$(4.3.19) \qquad E_{n+1}(f) = -\frac{2}{\pi} \sin \pi\varphi \int_0^{\infty} (2 \sinh^2 \theta/2)^{\varphi+\beta} (\cosh\theta+1)^{\alpha} \sinh\theta \times \times \frac{K_{\beta}(k\theta)}{I_{\beta}\, k\theta}\, d\theta .$$

From the asymptotic expression (4.3.17) it can be seen that the major contribution to the integral on the right of equation (4.3.19) comes from the neighbourhood of $\theta = 0$. Thus, on replacing $\sinh\theta$ by θ , $\cosh\theta$ by 1 , and using the asymptotic expression (4.3.17) for large k , equation (4.3.19) becomes

$$(4.3.20) \qquad E_{n+1}(f) \doteq -\frac{2\sin\pi\varphi}{2^{\varphi+\beta-\alpha}}\int_0^\infty \theta^{2(\beta+\varphi)+1} e^{-2k\theta}\, d\theta \; .$$

Finally putting $t = 2k\theta$ in equation (4.3.20) we obtain

$$(4.3.21) \qquad E_{n+1}(f) \doteq \frac{-2\sin\pi\varphi}{2^{\varphi+\beta-\alpha}(2k)^{2(\beta+\varphi+1)}}\,\Gamma[2(\beta+\varphi+1)] \; .$$

For $\varphi = \frac{1}{2}, \alpha = \beta = 0,$ we have the estimate

$$(4.3.22) \qquad E_{n+1}(f) \doteq \frac{-2.(2)^{1/2}}{(2n+3)^3} \; .$$

We compare the estimate (4.3.22) with the actual remainder term in Table 4.3.2. The estimated values are not as close to the actual values as in the previous example. A more careful analysis would, no doubt, give closer estimates but our estimates are close enough for practical purposes.

TABLE 4.3.2

Comparison of actual and estimated remainder terms in the numerical integration of $\int_{-1}^{1} (1+x)^{1/2}\,dx = 4\sqrt{2}/3$ using Gauss-Legendre Quadrature

n	Actual $R_{n+1}(f)$	Estimated $R_{n+1}(f)$
2	-0.007107	-0.008246
4	-0.001782	-0.002125
6	-0.000697	-0.000838
8	-0.000342	-0.000412
10	-0.000192	-0.000232

In a more general case when $f(x)$ is of the form $(x+1)^{\varphi} g(x)$ we would expand $f(x)$ as

$$(4.3.23) \qquad f(x) = (1+x)^{\varphi}\left[g(-1) + (1+x)g'(-1) + \frac{1+x^2}{2!} g''(-1) + \ldots \right].$$

This will give us an expression for $E_{n+1}(f)$ in terms of an infinite sum. In fact it is easily shown using equations (4.3.23) and (4.3.21) that

$$(4.3.24) \qquad E_{n+1}(f) = \frac{-2\sin \pi\varphi}{2^{(\varphi+\beta-\alpha)}\,2k^{2(\beta+\varphi+1)}} \times$$

$$\times \sum_{r=0}^{\infty} \frac{(-1)^r}{2} \frac{\Gamma[2(\beta+\varphi+1+r)]}{(2k)^r\, r!} \cdot g^{(r)}(-1) .$$

The infinite series in equation (4.3.24) is, in general, an asymptotic series and would therefore have to be terminated after a finite number of terms with the addition of an appropriate error term. However to estimate $E_{n+1}(f)$ it will usually be sufficient to take the first few terms of the infinite sum.

When $f(z)$ has a branch point on the real axis

Suppose that $f(z)$ has a branch point at the point $z = -d$, $d > 1$, on the real axis and that this is the only singularity of $f(z)$ in the finite part of the complex plane. Then we cut the plane along the real interval $(-\infty, -d)$.

The contour is similar to that described above in the case when $f(z)$ has a branch point at $z = -1$ with the point $-d$ taking the role of -1.

Again let us assume that the integral around $\mathcal{E}_\rho$ tends to zero as we let ρ tend to infinity. Also let us suppose that $f(z)$ is such that the integral around the semi-circles above and below the point $z = -d$ tends to zero with the radii of the semi-circles.

In this case the first asymptotic expression (4.3.2) may be used. We recall that $(z-1)^\alpha$ and $(z+1)^\beta$ were defined such that $|\arg(z-1)| < \pi$ and $|\arg(z+1)| < \pi$. Therefore equation (4.3.12) takes the form

$$E_{n+1}(f) = \int_{-\infty}^{-d} \left[K(x+0i)f(x+0i) - K(x-0i)f(x-0i)\right] dx. \tag{4.3.25}$$

Substituting the expression (4.3.4) into equation (4.3.25) and again putting $-x = \cosh\theta$ equation (4.3.25) gives us

$$E_{n+1}(f) = i \int_{\delta}^{\infty} \frac{(\cosh\theta+1)^{\alpha}(\cosh\theta-1)^{\beta}\sinh\theta}{e^{2n+\alpha+\beta+3}} \times \tag{4.3.26}$$

$$\times \left[e^{i\pi(\alpha+\beta)} f(-\cosh\theta+0i) - e^{-i\pi(\alpha+\beta)} f(-\cosh\theta-0i)\right] d\theta$$

where $\cosh\delta = d.$

We may approximate to the integral on the right using the process described above.

<u>Example</u>: Take $f(x) = (x+d)^{\varphi}$ where $d > 1$. Then

$$e^{i\pi(\alpha+\beta)} f(x+0i) - e^{-i\pi(\alpha+\beta)} f(x-0i) = 2i \sin\pi(\varphi+\alpha+\beta)(x+d)^{\varphi}. \tag{4.3.27}$$

Substituting equation (4.3.27) into equation (4.3.26) we have

$$E_{n+1}(f) = -2\sin\pi(\varphi+\alpha+\beta) \int_{0}^{\infty} \frac{(\cosh\theta+1)^{\alpha}(\cosh\theta-1)^{\beta}\sinh\theta}{e^{(2n+\alpha+\beta+3)\theta}} \times \tag{4.3.28}$$

$$\times \left[2\sinh\frac{\theta+\delta}{2}\sinh\frac{\theta-\delta}{2}\right]^{\varphi} d\theta.$$

Assuming the major contribution to $E_{n+1}(f)$ to come from the neighbourhood of $\theta = \delta$ equation (4.3.28) finally gives us

$$(4.3.29) \quad E_{n+1}(f) \doteq \frac{-2\sin\pi(\varphi+\alpha+\beta)(\delta^2-1)^{\frac{1+\varphi}{2}}(\delta+1)^{\alpha}(\delta-1)^{\beta}}{(2n+\alpha+\beta+3)^{1+\varphi}} \times \frac{\Gamma(1+\varphi)}{\left[\delta+(\delta^2+1)^{1/2}\right]^{2n+\alpha+\beta+3}} .$$

4.3(c) When $f(z)$ is an Entire Function of z

When $f(z)$ is an entire function of z then the remainder term, from equation (4.2.10), is given by

$$(4.3.30) \quad R_{n+1}(f) = \frac{1}{2\pi i}\int_{\mathcal{E}_\rho} \frac{\Pi_{n+1}^{(\alpha,\beta)}(z)}{P_{n+1}^{\alpha,\beta}(z)} f(z)\, dz$$

where $\mathcal{E}_\rho$ is any ellipse with foci at $+1$ and -1 surrounding the interval $[-1, 1]$. Using equation (4.3.4) the corresponding expression for $E_{n+1}(f)$ is given by

$$(4.3.31) \quad E_{n+1}(f) = \frac{1}{i}\int_{\mathcal{E}_\rho} \frac{(z-1)^{\alpha}(z+1)^{\beta}}{\left[z+(z^2-1)^{1/2}\right]^{2n+\alpha+\beta+3}} \cdot f(z)\, dz .$$

To estimate $E_{n+1}(f)$ we may be able to use either the minimisation technique or the saddle point method of Section 4.2(c).

4.3(c)(i) Upper Bounds on $|E_{n+1}(f)|$ over $\mathcal{E}_\rho$

On the ellipse $\mathcal{E}_\rho$ we have $|z+(z^2-1)^{1/2}| = \rho > 1$. Also for z on $\mathcal{E}_\rho$ we have the following upper bounds:

$$(4.3.32) \qquad |Z \pm 1|^{\gamma} = \begin{cases} (a+1)^{\gamma}, & \gamma > 0, \\ (a-1)^{\gamma}, & \gamma < 0, \end{cases}$$

where a $\left(a = \frac{1}{2}(\rho + 1/\rho) \right)$ is the semi-major axis of the ellipse $\mathcal{E}_{\rho}$.

Furthermore the length of the boundary of the ellipse is certainly less than that of a circle of radius a .

Therefore if $M(\rho)$ is an upper bound on $f(Z)$ for Z on $\mathcal{E}_{\rho}$ equation (4.3.21) gives us

$$(4.3.33) \qquad |E_{n+1}(f)| \leq \frac{2\pi a\,(a+1)^{\alpha+\beta}}{\rho^{2n+\alpha+\beta+3}} \cdot M(\rho)$$

when α and β are both positive. A similar result holds for α and β negative.

Now from the Maximum Modulus theorem $|f(Z)|$ takes its maximum value for Z in the region bounded by $\mathcal{E}_{\rho}$ on $\mathcal{E}_{\rho}$ itself. Thus $M(\rho)$ increases as we let ρ increase. The factor $\mathcal{F}(\rho) = 2\pi(a+1)^{\alpha+\beta} / \rho^{2n+\alpha+\beta+3}$ however decreases with ρ . The best estimate for $|E_{n+1}(f)|$ is that which makes the product $\mathcal{F}(\rho) . M(\rho)$ a minimum.

As we have already indicated the choice of ρ is usually selected from a finite set of values. The quantity $\mathcal{F}(\rho)$ need be calculated only once for all functions.

In Table 4.3.3 we tabulate $\mathcal{F}(\rho)$ for selected values of the semi-major axis, a , of the ellipse $\mathcal{E}_\rho$ corresponding to the Gauss-Legendre quadrature formulae $(\alpha = \beta = 0)$ with 3, 5, 7, 9 and 10 abscissae.

In the cases of the 3, 7 and 10 point formulae we compare these values with the corresponding values for Davis' bounds obtained from the tables of Lo, Lee and Sun [10] . To obtain a direct comparison of the upper bounds using the same value of $M(\rho)$ each entry in the tables of Lo, Lee and Sun has been multiplied by the factor $\sigma_\rho (\pi a b)^{1/2}$, see Davis and Rabinowitz [9, equation (30)] .

From an examination of the values of $\mathcal{F}(\rho)$ and Davis' factor, $\sigma_\rho (\pi a b)^{1/2}$, appearing in Table 4.3.3 it appears that $\mathcal{F}(\rho)$ is less than $\sigma_\rho (\pi a b)^{1/2}$ by factors $1/2$, $1/3$ and $1/4$ in the 3, 7 and 10 point Gauss-Legendre quadrature formulae respectively for each value of $a(\rho)$. In each case the upper bounds on the remainder term would therefore be less by a corresponding factor.

Table 4.3.3 was used to obtain upper bounds for the remainder term in the numerical integration of $exp(kx)$ over $[-1, 1]$ using Gauss-Legendre quadrature.

TABLE 4.3.3

Values of $\mathcal{J}(\rho)$ for use in obtaining upper bounds in Gauss-Legendre Quadrature:
A comparison with corresponding results of Davis

$a(\rho)$ \ $n+1$	3	3 (Davis)	5	7	7 (Davis)	9	10	10(Davis)
1.5	.(1)1119	.(1)2377	.(3)2383	.(5)5073	.(4)1638	.(6)1080	.(7)1575	.(7)6077
2.0	.(2)1248	.(2)3349	.(5)6433	.(7)3316	.(6)1154	.(9)1709	.(10)1227	.(10)5103
2.5	.(3)2714	.(3)6393	.(6)5149	.(9)9771	.(8)3499	.(11)1854	.(13)8077	.(12)3455
3.0	.(4)8261	.(3)1974	.(7)7159	.(10)6203	.(9)2253	.(13)5376	.(14)1582	.(14)6867
3.5	.(4)3100	.(4)7464	.(7)1404	.(11)6362	.(10)2345	.(14)2883	.(16)6136	.(15)2684
4.0	.(4)1342	.(4)3250	.(8)3494	.(12)9094	.(11)3347	.(15)2367	.(17)3819	.(16)1679
4.5	.(5)6465	.(4)1570	.(8)1036	.(12)1661	.(12)6134	.(16)2662	.(18)3370	.(17)1487
5.0	.(5)3378	.(5)8226	.(9)3518	.(13)3663	.(12)1356	.(17)3815	.(19)3894	.(18)1722
5.5	.(5)1883		.(9)1330	.(14)9392		.(18)6633	.(20)5575	
6.0	.(5)1107		.(10)5489	.(14)2722		.(18)1350	.(21)9509	
6.5	.(6)6796		.(10)2437	.(15)8739		.(19)3133	.(21)1876	
7.0	.(6)4331		.(10)1151	.(15)3058		.(20)8126	.(22)4189	
7.5	.(6)2850		.(11)5731	.(15)1152		.(20)2317	.(22)1039	
8.0	.(6)1927		.(11)2988	.(16)4631		.(21)7178	.(23)2826	
8.5	.(6)1336		.(11)1621	.(16)1968		.(21)2390	.(24)8327	
9.0	.(7)9452		.(12)9117	.(17)8793		.(22)8481	.(24)2634	
9.5	.(7)6818		.(12)5291	.(17)4105		.(22)3185	.(25)8873	
10.0	.(7)5003		.(12)3158	.(17)1994		.(22)1259	.(25)3163	

The figures in parenthesis denote the number of zeros between the decimal place and the first significant digit.
The number at the head of each column refers to the number of abscissae in the quadrature formula.

The upper bound on $|f(z)|$ for z on $\mathcal{E}_\rho$ is simply $\exp[k.a(\rho)]$ for $k > 0$. In Table 4.3.4 we illustrate how the most suitable choice of the upper bound is the minimum of a finite number of values of the product $\mathcal{F}(\rho).M(\rho)$.

TABLE 4.3.4

Product of $\mathcal{F}(\rho).\exp[k.a(\rho)]$

$a(\rho)$	$k=2, n=2$	$k=6, n=4$	$k=6, n=6$
1.5	0.225	1.931	0.0411
2.0	0.0681	<u>1.047</u>	0.00540
2.5	0.0403	1.683	<u>0.00319</u>
3.0	<u>0.0333</u>	4.700	0.00407
3.5	0.0340	18.52	0.00839
4.0	0.0400		
4.5	0.0523		
5.0	0.0744		

$a(\rho)$	$k=2, n=6$
5.5	0.(9)562
6.0	0.(9)443
6.5	0.(9)387
7.0	<u>0.(9)368</u>
7.5	0.(9)377
8.0	0.(9)411

(The figures in parenthesis denote the number of zeros between the decimal point and the first significant digit.)

The upper bounds so obtained are compared with the actual remainder term and the estimates of the next section in Table 4.3.5.

4.3(c)(ii) The Saddle Point Method

The saddle point method has been discussed in Section 4.2(c)(ii) and we shall illustrate the method here by use of an example.

Example: Consider the function $\exp(kx),\ k > 0$ and let us use the Gauss-Legendre quadrature formula.

The remainder term for large n is given asymptotically by

$$E_{n+1}(f) \doteq \frac{1}{i}\int_{\mathcal{E}_\rho} \frac{e^{kz}}{\left[z+(z^2-1)^{1/2}\right]^{2n+3}}\,dz \qquad (4.3.34)$$

Let us write the integrand in equation (4.3.34) in the form $\exp\left[\chi(z)\right]$ where

$$\left[\chi(z)\right] = kz - (2n+3)\log\left[z+(z^2-1)^{1/2}\right] . \qquad (4.3.35)$$

The integrand has saddle points where $\chi'(z) = 0$; that is, where

$$k - \frac{(2n+3)}{(z^2-1)^{1/2}} = 0 . \qquad (4.3.36)$$

From equation (4.3.36) we see that the saddle point is given by $Z = Z_0 = \left[1 + (2n+3)^2/k^2\right]^{1/2}$. We take the positive sign of the square root so that equation (4.3.36) may be satisfied.

The ellipse $\mathcal{E}_\rho$ is deformed to pass through the point $Z = Z_0$

Now for large values of n equation (4.3.35) gives us

$$\chi''(z_0) = \frac{(2n+3)\, z_0}{(z_0^2 - 1)^{3/2}} \tag{4.3.37}$$

$$= \frac{k^2}{(2n+3)^2}\left[(2n+3)^2 + k^2\right]^{1/2}.$$

Thus the line of steepest descent has unit vector α where

$$|\alpha| = 1 \quad , \quad \arg\alpha = \tfrac{1}{2}\pi - \tfrac{1}{2}\arg\left[\chi''(z)\right] \tag{4.3.38}$$

or

$$\alpha = i \quad . \tag{4.3.38A}$$

As we leave the saddle point in a direction perpendicular to the real axis (the line of steepest descent) $\exp(kz)$ decreases rapidly. We may then assume that the major contribution to $E_{n+1}(f)$ comes from that part of the contour in the neighbourhood of the saddle point.

Substituting into equation (4.2.19) we finally obtain

$$(4.3.39)\quad E_{n+1}(f) \sim \frac{(2\pi)^{1/2}\, k^{2n+2}\,(2n+3)\; e^{[k^2+(2n+3)^2]^{1/2}}}{[(2n+3)^2+k^2]^{1/4}\,\left\{2n+3+[(2n+3)^2+k^2]^{1/2}\right\}^{2n+3}} .$$

In Table 4.3.5 we compare the actual remainder term with the estimate (4.3.38) and the upper bound given by the inequality (4.3.33) for $k = 2$ and 6. In each case it appears that the upper bounds are greater than the asymptotic estimates by a factor of 10. The extra effort in using the saddle point seems therefore to be worthwhile.

TABLE 4.3.5

Actual and estimated values together with upper bounds for the remainder in the numerical integration of $\int_{-1}^{1} e^{kx}\,dx$ using Gauss-Legendre quadrature

	n	$\{R_{n+1}(f)\}$ Actual	Asymptotic Estimates	Upper Bounds
$k=2$	2	0.(2)46	0.(2)498	0.(1)33
	4	0.(6)91	0.(6)938	0.(5)75
	6	*	0.(10)377	0.(9)368
	8	*	0.(15)508	0.(14)557
$k=6$	2	8.36	9.21	89.7
	4	0.100	0.109	1.04
	6	*	0.(3)301	0.(2)319
	8	*	0.(6)298	0.(5)352

*To the number of digits with which we were working the actual remainders were insignificant.

4.3(d) When $f(z)$ has an essential singularity at -1

Let us suppose that $f(z)$ has an essential singularity at the end point -1 and that $f(z)$ tends to a unique limit as z tends to -1 in the sector $|\arg(z-1)| < \beta$. Then the contour may be taken to be that depicted in Fig. 4.2.

The integrals around the arcs at ± 1 tend to zero with the radii of the arcs and the contribution from the parallel lines joining b to Γ_ρ cancel.

To estimate the integral along Γ_ρ we use the saddle point method described in Section 4.3(c)(ii).

Example: Consider the function $\exp[-1/(1+x)]$ and let us use the Gauss-Legendre quadrature formula.

From equation (4.3.4) the remainder term is given asymptotically for large n by

$$(4.3.40) \qquad E_{n+1}(f) = \frac{1}{i}\left\{\int_{c^+} + \int_{c^-}\right\} \frac{e^{-\frac{1}{z+1}}}{[z+(z^2-1)^{1/2}]^{2n+3}}\, dz \quad .$$

Following Section 4.3(c)(ii) we have

$$(4.3.41) \qquad \chi(z) = -\frac{1}{z+1} - (2n+3)\log[z+(z^2-1)^{1/2}] \quad .$$

The saddle points are therefore the solutions of the equation

(4.3.42) $$\frac{1}{(Z+1)^2} = \frac{(2n+3)}{(Z^2-1)^{1/2}} .$$

If we assume that the solutions of equation (4.3.42) are close to -1 we find that the saddle points Z_1 and Z_2 (say), are given by

(4.3.43) $$Z_1 = -1 + \left(\frac{2^{1/2}}{2n+3}\right)^{2/3} e^{i\pi/3}$$

and

(4.3.44) $$Z_2 = -1 + \left(\frac{2^{1/2}}{2n+3}\right)^{2/3} e^{-i\pi/3} .$$

Also from equation (4.3.41) we have

(4.3.45) $$\chi''(Z) = -\frac{2}{(Z+1)^3} + \frac{(2n+3)\,Z}{(Z^2-1)^{3/2}} .$$

From equation (4.3.45) it is easily shown that $\chi''(Z_1)$ and $\chi''(Z_2)$ are both asymptotically equal to $(2n+3)^2$. Thus from equation (4.2.20) and an examination of the direction of the contours we find $\alpha_1 = \alpha_2 = -i$ where α_1 and α_2 are unit vectors along the lines of steepest descent through Z_1 and Z_2 respectively.

From equation (4.3.42) we see that $z_1+(z_1^2-1)^{1/2} = z_1+(2n+3)(z_1+1)^2$.
Therefore using equation (4.3.33) we have

$$(4.3.46) \qquad \left[z_1+(z_1^2-1)^{1/2}\right]^{-(2n+3)} = -\left[1-\frac{2^{1/3}e^{i\pi/3}}{(2n+3)^{2/3}}-\frac{2^{2/3}e^{2i\pi/3}}{(2n+3)^{1/3}}\right]^{-(2n+3)}$$

$$= -\left[1-\frac{2^{2/3}e^{2i\pi/3}}{(2n+3)^{1/3}}+O\left(\frac{1}{(2n+3)^{2/3}}\right)\right]^{-2n+3}.$$

For large n equation (4.3.46) gives us

$$(4.3.47) \qquad \left[z_1+(z_1^2-1)^{1/2}\right]^{-2n-3} \sim -\exp\left[2^{2/3}(2n+3)^{2/3}e^{2i\pi/3}\right].$$

Similarly we find

$$(4.3.48) \qquad \left[z_2+(z_2^2-1)^{1/2}\right]^{-2n-3} \sim -\exp\left[2^{2/3}(2n+3)^{2/3}e^{-2i\pi/3}\right].$$

Taking the major contribution to the remainder term to come from that part of the contour passing through the saddle points equations (4.2.19) and (4.3.40) finally give us

$$(4.3.49) \qquad E_{n+1}(f) \sim \frac{2(2\pi)^{1/2}}{2n+3}\exp\left[-3\left(\frac{2n+3}{4}\right)^{2/3}\right]\cos\left[3^{3/2}\left(\frac{2n+3}{4}\right)^{2/3}\right].$$

We compare this estimate with the actual remainder in Table 4.3.6.

TABLE 4.3.6

Actual and Estimated errors in evaluating
$\int_1^1 exp[-1/(1+x)]\,dx = 0.6532877\ldots$ using
Gauss-Legendre quadrature.

n	Actual $R_{n+1}(f)$	Estimated $R_{n+1}(f)$
2	0.00348	0.00278
4	-0.000906	-0.000903
6	0.000231	0.000239
8	-0.000026	-0.000028
10	-0.000008	-0.000008

4.4 Gauss-Laguerre Quadrature Formulae

From equation (2.4.11) the remainder term in the Gauss-Laguerre quadrature formula is given by

$$(4.4.1) \qquad R_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{C^+} + \int_{C^-}\right\} \frac{\Lambda_{n+1}^{(\alpha)}(z)}{L_{n+1}(z)} f(z)\,dz$$

where the contours C^+ and C^- at the end point 0 are as described in the fundamental theorem while at the infinite end point we may consider the contours to be asymptotic to the real axis.

The ratio $\Lambda_{n+1}^{(\alpha)}(z) / L_{n+1}^{(\alpha)}(z)$ has no singularities in the finite part of the complex plane cut along $[0,\infty)$. Therefore the behaviour at the end point 0 of C^+ and C^- is similar to that described in Section 4.2 of this chapter.

Suitable asymptotic expressions for $\Lambda_{n+1}^{(\alpha)}(z)$, $L_{n+1}^{(\alpha)}(z)$ are given by Elliott and Robinson [41, equations (3.11) and (5.12)]. We have, for large n,

$$L_{n+1}^{(\alpha)}(z) \sim \frac{1}{2\pi^{1/2}} \cdot (-z)^{-\alpha/2-1/4}(n+1)^{\alpha/2-1/4} e^{z/2} e^{2(n+1)^{1/2}(-z)^{1/2}} \tag{4.4.2}$$

and

$$\Lambda_{n+1}^{(\alpha)}(z) \sim -\pi^{1/2}\left(n+1+\frac{\alpha+1}{2}\right)^{\alpha/2-1/4}(-z)^{\alpha/2-1/4} e^{-z/2} e^{-2\left(n+1+\frac{\alpha+1}{2}\right)^{1/2}(-z)^{1/2}} \tag{4.4.3}$$

for $|z|$ bounded and not in $[0, \infty)$. In the expressions (4.4.2) and (4.4.3) we take that branch of $(-z)^{\alpha}$ specified by $|\arg(-z)| < \pi$. From these expressions we have

$$K(z) = -2\pi\left[1+\frac{\alpha+1}{2(n+1)}\right]^{\alpha/2-1/4} e^{-z}(-z)^{\alpha} e^{-2\left[\left(n+1+\frac{\alpha+1}{2}\right)^{1/2}+(n+1)^{1/2}\right](-z)^{1/2}}. \tag{4.4.4}$$

Now the most significant factor, for large n, and $|z|$ bounded on the right of equation (4.4.4) is $\exp\left\{-2\left[\left(n+1+\frac{\alpha+1}{2}\right)^{1/2}+(n+1)^{1/2}\right](-z)^{1/2}\right\}$. The curves in this case would then be taken to be those defined by $Re[(-z)^{1/2}] = \rho > 0$.

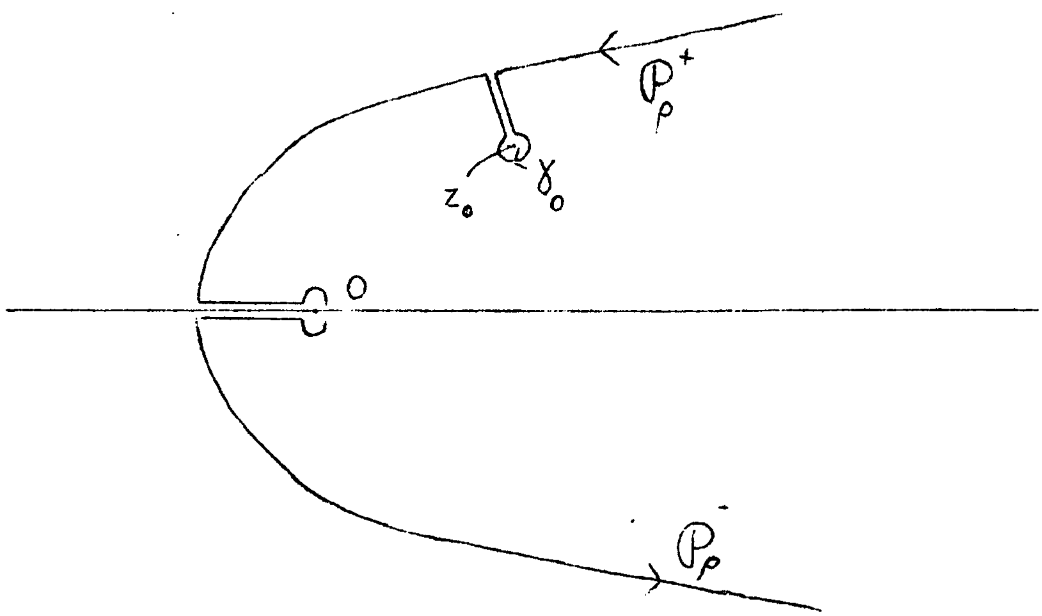
The curve, $Re\,[(-z)^{1/2}] = \rho$, is one of a family of parabolae $\mathcal{P}_\rho$, say, whose common focus is the origin. When $\rho = 0$ we have the degenerate parabola, the real interval $[0, \infty)$.

The parabola $\mathcal{P}_\rho$ extends to infinity where the asymptotic expression (4.4.4) is not valid. However in many cases the major contribution to the remainder term will come from the finite part of the plane where we may use this expression.

4.4(a) When $f(z)$ is a meromorphic function

Suppose that $f(z)$ has a simple pole at $z = z_0$ and that this is the only singularity of $f(z)$ in the finite part of the complex plane. Then we may take the contours C^+ and C^- to be those depicted in Fig. 4.1 except that the curves $\mathcal{P}_\rho^{\pm}$ are not closed curves, see Fig. 4.3.

FIGURE 4.3



Following Section 4.2(a) the major contribution to the integral comes from the integral around the small circle γ_0 provided that we can show that the integral along C_ρ is small for large values of ρ. Thus from equation (4.4.4) and equation (4.2.4) we obtain

$$(4.4.5) \quad E_{n+1}(f) = 2\pi\left[1+\frac{\alpha+1}{2(n+1)}\right]^{\alpha/2-1/4} e^{-z_0}(-z_0)^{\alpha} e^{-2\left[(n+1+\frac{\alpha+1}{2})^{1/2}+(n+1)^{1/2}\right](-z_0)^{1/2}} \cdot g(z_0)$$

where $g(z_0)$ is the residue of $f(z)$ at $z = z_0$.

The result can of course be immediately extended to more than one simple pole and to poles of order more than 1.

4.4(b) When $f(z)$ has a branch point at the origin

When $f(z)$ has a branch point at the origin we cut the plane along the negative real axis. The asymptotic expression (4.4.4) is not valid at the origin. However we obtain from Elliott and Robinson [42] the asymptotic expression

$$(4.4.6) \quad K_1(z) = -2e^{-z}(-z)^{\alpha} \frac{K_\alpha\left\{\left[4(n+1)+(2\alpha+2)\right]^{1/2}(-z)^{1/2}\right\}}{I_\alpha\left\{\left[4(n+1)+(2\alpha+2)\right]^{1/2}(-z)^{1/2}\right\}},$$

$|\arg(-z)| < \pi$, which is valid for $|z|$ bounded including the origin.

Again if we can show that the contribution from $\mathcal{C}_\rho$ for large ρ is small, equation (4.2.9) gives us

$$(4.4.7) \quad E_{n+1}(f) = -\frac{1}{\pi i}\int_{-\rho^2}^{0} e^{-x}(-x)^{\alpha}\, \frac{K_\alpha\{[4(n+1)+2\alpha+2]^{1/2}(-z)^{1/2}\}}{I_\alpha\{[4(n+1)+2\alpha+2]^{1/2}(-z)^{1/2}\}} \times$$

$$\times\, [\, f(x+0i) - f(x-0i)]\, dx \quad .$$

where $-\rho^2$ is the point of intersection of $\mathcal{C}_\rho$ and the negative real axis. We cannot let ρ tend to infinity immediately since the integral in equation (4.4.7) is not in general convergent.

<u>Example:</u> Let us take $f(x) = \log x$. In Section 2.3 we did not consider explicitly a function with a logarithmic singularity at the end point of the range. However, the arguments for such a singularity do not differ from those for an algebraic singularity.

In this example we have

$$(4.4.8) \qquad f(x+0i) - f(x-0i) = 2\pi i \, .$$

Thus equation (4.4.7) gives us

$$(4.4.9) \quad E_{n+1}(f) = -2\int_{-\rho^2}^{0} e^{-x}(-x)^{\alpha}\, \frac{K_\alpha[N(-x)^{1/2}]}{I_\alpha[N(-x)^{1/2}]}\, dx \, .$$

where $N = [4(n+1)+2\alpha+2]^{1/2}$. Now for large N $K_\alpha[N(-x)^{1/2}]/I_\alpha[N(-x)^{1/2}] \sim \pi e^{-2N(-x)^{1/2}}$, and equation (4.4.9) then gives us

$$(4.4.10) \quad E_{n+1}(f) \doteq -2\pi \int_{-\rho^2}^{0} (-x)^{\alpha} e^{-x-2N(-x)^{1/2}} dx ,$$

For fixed ρ and large N the major contribution to the integral on the right of the expression (4.4.10) comes from the neighbourhood of $x = 0$ so that

$$(4.4.11) \quad E_{n+1}(f) \doteq -2\pi e^{0} \int_{-\rho^2}^{0} (-x)^{\alpha} e^{-2N(-x)^{1/2}} dx$$

$$\doteq -2\pi e^{0} \int_{-\infty}^{0} (-x)^{\alpha} e^{-2N(-x)^{1/2}} dx .$$

Putting $t = 2N(-x)^{1/2}$ in equation (4.4.11) we obtain finally

$$(4.4.12) \quad E_{n+1}(f) \doteq - \frac{\pi \, \Gamma(2\alpha+2)}{2^{2\alpha}\left[4(n+1)+2\alpha+2\right]^{\alpha+1}} .$$

For $\alpha = 0$ the approximation (4.4.12) gives us

$$(4.4.13) \quad E_{n+1}(f) \doteq - \frac{\pi}{\left[4(n+1)+2\right]}$$

The actual and estimated remainder terms relevant to $f(x) = \log x$ using the Gauss-Laguerre quadrature formulae are compared in Table 4.4.1.

TABLE 4.4.1

Actual and estimated values of the remainder term in the numerical integration of $\int_0^\infty e^{-x} \log dx$ using Gauss-Laguerre quadrature formulae

n	$\sum_{k=0}^{n} \lambda_{k,n} f(x_{k,n})$	Actual $R_{n+1}(f)$	Estimated $R_{n+1}(f)$
2	-0.37379	-0.203	-0.224
4	-0.45362	-0.123	-0.142
6	-0.48845	-0.089	-0.105
8	-0.50819	-0.069	-0.082

4.4(c) When $f(z)$ is an entire function of z

When $f(z)$ is an entire function of z it does not appear easy to use the minimisation technique described in Section 4.2(c)(i). The difficulty of course lies in the fact that the length of the parabola is not finite.

We should, however, be able to use the saddle point method to advantage.

The Saddle Point Method

Using the asymptotic expression (4.4.4) for the ratio $\psi(z)/\phi(z)$ we proceeded formally with the saddle point method to obtain

estimates of the remainder term in the application of Gauss-Laguerre formulae to the numerical integration of $\int_0^\infty x^\alpha e^{-x} e^{-x} dx$.
The estimated values when compared with the actual values were not satisfactory.

It appears that more care must be exercised here than in the case of the Gauss-Legendre quadrature formulae. The saddle point ζ (say) is such that $|\zeta|$ increases with increasing n. We must then use an asymptotic expression which is valid for both n and $|\zeta|$ large while the expressions (4.4.4) and (4.4.7) are valid only for $|\zeta|$ bounded.

The functions $L_{n+1}^{(\alpha)}(z)$ and $\Lambda_{n+1}^{(\alpha)}(z)$ are known in terms of the confluent hypergeometric functions, see Section 5.3, and asymptotic expansions for these last functions for both $|\zeta|$ and n large are given in Slater [43, Chapt.4]. However an examination of the corresponding asymptotic expansions for $L_{n+1}^{(\alpha)}(z)$ and $\Lambda_{n+1}^{(\alpha)}(z)$ indicate that it is not sufficient to consider the first term only of these expansions.

Explicit expressions for the successive terms of the expansion (given by Slater [43, Sect. 4.6.2] in terms of recurrence relations) have yet to be obtained. We shall therefore defer any further discussion of this problem to a later date.

4.5 Gauss-Hermite Quadrature Formulae

In the Gauss-Hermite quadrature formulae the contours C^+ and C^- extend to infinity in both the positive and negative directions.

The required asymptotic expression for the ratio $\eta_{n+1}(z)/H_{n+1}(z)$ from Elliott and Robinson [41, equations (6.12) and (6.13)] is found to be given by

$$K(z) = (2\pi)(-1)^n e^{\mp i\pi/2} e^{-z^2} e^{\pm 2(2n+4)^{1/2} z i} \tag{4.5.1}$$

where the upper signs are taken for $Im(z) > 0$ and the lower signs for $Im(z) < 0$.

Again this expression is only valid for $|z|$ bounded. We consider however, in the first instance, only that part of C^+ and C^- in the finite part of the complex plane.

On examination of equation (4.5.1) we find that the curves Γ_ρ would be taken to be the straight lines, S_ρ (say), defined by $|Im(z)| = \rho > 0$. The family of curves consists then of pairs of lines parallel to and equidistant from the real axis.

4.5(a) When $f(z)$ is a meromorphic function

Corresponding to the previous sections on meromorphic functions we find that, when $f(z)$ has a simple pole at $z = z_0$, $Im(z_0) > 0$,

$$E_{n+1}(f) = -2\pi e^{-i\pi/2}(-1)^n e^{-z_0^2} e^{2(2n+4)^{1/2} z_0 i} \cdot g(z_0) \tag{4.5.2}$$

where $g(z_0)$ is the residue of $f(z)$ at $z = z_0$.

We compare the actual and estimated errors corresponding to the function $1/(1+x^2)$ in Table 4.5.1. The actual errors were obtained from a paper by Rosser [44].

TABLE 4.5.1

Actual and estimated values of the remainder term in the numerical integration of $\int_{-\infty}^{\infty} e^{-x^2}/(1+x^2)\, dx$ using Gauss-Hermite quadrature formulae

	Actual $R_{n+1}(f)$	Estimated $R_{n+1}(f)$
1	+0.16	+0.13
9	+0.0016	+0.0014
15	+0.00016	+0.00015

There is no result corresponding to a singularity of $f(z)$ at an end point. However when $f(z)$ is an entire function we may be able to use the saddle point method.

The Saddle Point Method

As for the Gauss-Laguerre formula the functions relevant to the Hermite formula, $H_{n+1}(z)$ and $\eta_{n+1}(z)$, are known in terms of the confluent hypergeometric function. The comments that were made in Section 2.4(c) also apply to the Hermite quadrature formula.

4.6 Newton-Cotes Quadrature Formula

In the case of the Newton-Cotes quadrature formula the remainder term $R^{x}_{n+1}(f)$ which includes the contribution from the end points is given by equation (2.4.30). We have

$$(4.6.1) \qquad R^{x}_{n+1}(f) = \frac{1}{2\pi i}\left\{\int_{c^+} + \int_{c^-}\right\} \frac{q_{n+1}(z)}{p_{n+1}(z)}\, f(z)\, dz \quad .$$

Again the ratio $q_{n+1}(z)/p_{n+1}(z)$ is analytic in the complex plane cut along the interval of integration. We may then follow Section 4.2 closely.

Let us take the interval of integration to be $[-1, 1]$.

In Chapter III we developed an asymptotic expression for the ratio $q_{n+1}(z)/p_{n+1}(z)$ which is valid for all z except in a neighbourhood of $[-1, 1]$. From equation (3.2.22) and equation (3.1.11) we find

$$K(z) = -\frac{4(2\pi)^{1/2}(z^2-1)^{-1/2}}{n^{3/2}[(\log n)^2+\pi^2]}\left[\frac{1}{z-1}-\frac{(-1)^n}{z+1}\right] \times \tag{4.6.2}$$
$$\times\left\{\exp\left[\frac{z+1}{2}\log(z+1)-\frac{z-1}{2}\log(z-1)-\log 2\right]\right\}^{-n}.$$

The curves Γ_ρ are in this case defined by the equation, see equation (3.2.24),

$$Rl\left[\frac{z+1}{2}\log(z+1)-\frac{z-1}{2}\log(z-1)-\log 2\right] = \rho > 0 . \tag{4.6.3}$$

We shall denote these curves by $\mathcal{C}_\rho$. The family of curves is depicted in Fig. 3.1.

4.6(a) When $f(z)$ is a meromorphic function

Suppose that the only singularity in the finite complex plane of $f(z)$ is a simple pole at the point $z = z_0$. Then the contours C^+ and C^- take the form depicted in Fig. 4.1 where the curve Γ_ρ is one of the family $\mathcal{C}_\rho$.

In this case the integral around the small semi-circles at $+1$ and -1 do contribute since $p_{n+1}(z)$ has zeros at these points. We add this contribution to the quadrature sum.

As in the previous cases, if we can show that the contribution from the integral along $\mathscr{C}_\rho$ tends to zero as we let ρ increase then the remainder term is the integral around γ_0.

Thus from equation (4.2.4) we have

$$(4.6.4) \qquad E_{n+1}(f) = -K(z_0) \,.\, g(z_0)$$

where $g(z_0)$ is the residue of $f(z)$ at $z = z_0$ and $K(z)$ is defined by equation (4.6.2).

<u>Example</u>: Consider the function $f(z) = 1/(1+z^2)$. The residues of $f(z)$ at the simple poles $+1$ and -1 are $1/2i$ and $-1/2i$ respectively.

We may show that the integral around $\mathscr{C}_\rho$ tends to zero as we let ρ increase as follows.

Let $a(\rho)$ be the positive intercept of $\mathscr{C}_\rho$ with the positive x-axis; $a(\rho)$ tends to infinity with ρ.

For large ρ the factors $(z \pm 1)$ are approximately equal to $a(\rho)$. Also the length of the curve is approximately that of a circle of radius $a(\rho)$. Therefore from equation (4.6.2) we have for large ρ

$$(4.6.5)\qquad |E_{n+1}(f, \ell_\rho)| \le \frac{4(2\pi)^{1/2}}{n^{3/2}[(\log n)^2+\pi^2]} \cdot \frac{2}{[a(\rho)]^2}\, e^{-n\rho}\, 2\pi a(\rho).$$

The right hand side of the inequality (4.6.5) obviously tends to zero as ρ increases.

Therefore, for large n , we have from equation (4.6.4)

$$(4.6.6)\qquad E_{n+1}(f) = \frac{1}{2i}\left[K(-i) - K(i)\right] .$$

Using equation (4.6.2) we find, after a little algebra

$$(4.6.7)\qquad K(i) = \frac{2\pi^{1/2} 2^{n/2} e^{-n\pi/4} e^{in\pi/2} \{1+(-1)^n + i[1-(-1)^n]\}}{i\, n^{3/2}[(\log n)^2+\pi^2]}$$

and

$$(4.6.8)\qquad K(-i) = -\frac{2\pi^{1/2} 2^{n/2} e^{-n\pi/4} e^{in\pi/2} \{1+(-1)^n + i[1-(-1)^n]\}}{i\, n^{3/2}[(\log n)^2+\pi^2]} .$$

Substituting equations (4.6.7) and (4.6.8) into equation (4.6.6) we finally obtain

$$(4.6.9)\qquad E_{n+1}(f) = \frac{4\pi^{1/2} 2^{n/2} e^{-n\pi/4} \cos(n\pi/2)}{n^{3/2}[(\log n)^2+\pi^2]} .$$

We compare the actual and estimated values in Table 4.6.1.

TABLE 4.6.1

Actual and estimated values of the remainder term in the numerical integration of $\int_{-1}^{1} 1/(1+x^2).dx$ using Newton-Cotes quadrature formulae

n	Actual $R_{n+1}(f)$	Estimated $R_{n+1}(f)$
2	-0.0959	-0.1007
4	0.0108	0.0130
6	-0.00224	-0.00265
8	0.00057	0.00066
10	-0.00016	-0.00018

4.6(b) When $f(z)$ has a branch point at -1

The asymptotic expression (4.6.2) for $K(z)$ is not valid near -1 . Hence another asymptotic expression for $q_{n+1}(z) / p_{n+1}(z)$ must be found which is valid at that point.

As yet we have been unable to find a suitable one and we will defer the discussion of this problem.

4.6(c) When $f(z)$ is an entire function of z

Suppose $f(z)$ is an entire function of z . Then from equation (4.2.11) the quantity $E_{n+1}(f)$ is given by

$$(4.6.10) \qquad E_{n+1}(f) = \frac{1}{2\pi i} \int_C K(z)\, f(z)\, dz$$

where C is any contour surrounding the basic interval $[-1, 1]$ and $K(z)$ is defined by equation (4.6.2).

As in Section 4.2(c) we can use either the minimisation technique or the saddle point method to estimate $E_{n+1}(f)$.

4.6(c)(i) Upper bounds on $|E_{n+1}(f)|$

In this method we would take the contour C to be initially one of the curves $\mathcal{E}_\rho$ defined by equation (4.6.3).

Let us write

$$(4.6.11) \qquad K(z) = g(z) \cdot \exp\left[\frac{z+1}{2} \log(z+1) - \frac{z-1}{2} \log(z-1) - \log 2 \right]^{-n}$$

where

$$(4.6.12) \qquad g(z) = \frac{-4 \cdot (2\pi)^{\frac{1}{2}}}{n^{3/2}[(\log n)^2 + \pi^2]} \left[\frac{(z+1) - (-1)^n (z-1)}{(z^2-1)^{3/2}} \right].$$

Very little is known about the curve $\mathcal{E}_\rho$ and it would be extremely difficult to place upper bounds on $|g(z)|$ for z

on $\mathscr{C}_\rho$ and of course to place upper bounds on $|f(z)|$ itself. It is therefore more convenient to examine the circle $|z| = a(\rho)$ where $a(\rho)$ is the positive intercept of the curve $\mathscr{C}_\rho$ with the positive x-axis.

The curve $\mathscr{C}_\rho$ lies inside the circle $|z| = a(\rho)$. It is of some interest to note that in the limit as ρ tends to infinity $\mathscr{C}_\rho$ is a circle of infinite radius. In doing this we will increase the magnitude of the upper bounds but the analysis is considerably simplified.

Each point on $|z| = a(\rho)$ will lie on one of the curves $\mathscr{C}_{\rho'}$ where $\rho' \geq \rho$. Therefore for ζ on this circle we have

$$\text{(4.6.13)} \qquad Re\left[\frac{\zeta+1}{2}\log(\zeta+1) - \frac{\zeta-1}{2}\log(\zeta-1) - \log 2\right] \geq \rho \ .$$

Now let $M(\rho)$ be an upper bound for $f(z)$ on $a(\rho)$
Then using Schwarz's inequality equation (4.6.10) gives us

$$\text{(4.6.14)} \qquad |E_{n+1}(f)| \leq \frac{1}{2\pi}\int_{|z|=a(\rho)} |K(z)|\,.\,|f(z)|\,.\,|dz| \ .$$

Using equations (4.6.12) and (4.6.13) the inequality (4.6.14) becomes

$$\text{(4.6.15)} \qquad |E_{n+1}(f)| \leq \frac{M(\rho)\,.\,4(2\pi)^{1/2}e^{-n\rho}}{n^{3/2}\left[(\log n)^2+\pi^2\right]} \times$$

$$\times \ \frac{1}{2\pi}\int_{|z|=a(\rho)} \frac{|z+1-(-1)^n(z-1)|}{|z^2-1|^{3/2}}\,|dz| \ .$$

Let I denote the integral on the right of the inequality (4.6.15). Then substituting $z = a(\rho)\, e^{i\theta}$ we have

$$(4.6.16) \qquad I = \left\{ a(\rho)\left[1-(-1)^n\right] + 1 + (-1)^n \right\} \int_0^{2\pi} \frac{d\theta}{\left\{[a(\rho)]^4 + 1 - 2[a(\rho)]^2 \cos 2\theta\right\}^{3/4}}$$

$$\leq \left\{ a(\rho)\left[1-(-1)^n\right] + 1 + (-1)^n \right\} \cdot \frac{2\pi}{\left\{[a(\rho)]^2 - 1\right\}^{3/2}} \; .$$

Substituting the inequality (4.6.16) into (4.6.15) we obtain the desired upper bound

$$(4.6.17) \quad \left|E_{n+1}(f)\right| \leq M(\rho) . \mathcal{F}(\rho)$$

where

$$(4.6.18) \quad \mathcal{F}(\rho) = \frac{4(2\pi)^{1/2} e^{-n\rho}}{n^{3/2}\left[(\log n)^2 + \pi^2\right]} \cdot \frac{a(\rho)\left\{ a(\rho)\left[1-(-1)^n\right] + 1 + (-1)^n \right\}}{\left\{[a(\rho)]^2 - 1\right\}^{3/2}}$$

Our object is now to find that value of ρ which makes the right hand side of equation (4.6.17) a minimum. The factor $\mathcal{F}(\rho)$ defined by equation (4.6.18) may be computed for varying ρ once only for all functions. A table of such values, Table 4.6.2, is given below for the Newton-Cotes 3, 5, 7, 9 and 11 point formulae.

TABLE 4.6.2

Table of $\mathcal{F}(\rho)$ for use in obtaining upper bounds in Newton-Cotes Quadrature

$\alpha(\rho)$ \ $n+1$	3	5	7	9	11
1.5	.(0)2100	.(1)1865	.(2)2620	.(3)4489	.(4)8601
2.0	.(1)3896	.(2)1792	.(3)1303	.(4)1154	.(5)1146
2.5	.(1)1301	.(3)3699	.(4)1663	.(6)9123	.(7)5596
3.0	.(2)5661	.(3)1098	.(5)3369	.(6)1261	.(8)5275
3.5	.(2)2880	.(4)4062	.(6)9060	.(7)2465	.(9)7499
4.0	.(2)1626	.(4)1744	.(6)2959	.(8)6121	.(9)1416
4.5	.(3)9895	.(5)8350	.(6)1114	.(8)1813	.(10)3300
5.0	.(3)6377	.(5)4345	.(7)4680	.(9)6149	.(11)9036
5.5	.(3)4298	.(5)2415	.(7)2145	.(9)2323	.(11)2815
6.0	.(3)3005	.(5)1416	.(7)1055	.(10)9584	.(12)9740
6.5	.(3)2165	.(6)8679	.(8)5502	.(10)4254	.(12)3678
7.0	.(3)1600	.(6)5524	.(8)3016	.(10)2008	.(12)1496
7.5	.(3)1208	.(6)3630	.(8)1725	.(11)9998	.(13)6481
8.0	.(4)9294	.(6)2453	.(8)1024	.(11)5211	.(13)2967

The figures in parenthesis denote the number of zeros between the decimal place and the first significant digit.
The number at the head of each column refers to the number of abscissae in the quadrature formula.

A comparison of $\mathcal{F}(\rho)$ with Davis' factor $\sigma_\rho(\pi a b)^{\frac{1}{2}}$, [9, equation (10)], should not be made here because our contour is a circle while Davis' is an ellipse. However in many cases $|f(z)|$ takes its maximum value on the real axis and the upper bound $M(\rho)$ will in both cases be the same. (In general Davis' upper bound for $|f(z)|$ will be smaller than ours.) For such a function a direct comparison may be made. In Table 4.6.3 we compare values corresponding to Simpson's rule. We see from the table that our entries are a great deal larger for $a(\rho)$ near unity than Davis'; this is to be expected since our asymptotic expression is not valid in the neighbourhood of ± 1. However for large values of $a(\rho)$ our entries are less than the corresponding entries of Davis.

As in the case of Gauss-Legendre formulae we compare, in Table 4.6.4, the upper bounds obtained from Table 4.6.2 with the actual values and the asymptotic values (equation (4.6.26) of the remainder term in the numerical integration of e^{2x} over the interval $[-1, 1]$ using the Newton-Cotes integration formulae. The value of $M(\rho)$ is obviously $\exp[2a(\rho)]$.

The quantity in brackets in the last column of the table refers to the radius of the circle which gives the least upper bound.

Again we note that the upper bounds exceed the actual remainder by a factor of 10.

TABLE 4.6.3

Comparison of $\mathcal{F}(\rho)$ and Davis' $\sigma_\rho(\pi a b)^{1/2}$ for Simpson's Rule.

$a(\rho)$	$\mathcal{F}(\rho)$	$\sigma_\rho(\pi a b)^{1/2}$ (Lo, Lee, Sun [10])
1.1	5.224	1.681
1.5	0.210	0.2026
2.0	0.0389	0.0492
2.5	0.0130	0.0181
3.0	0.00566	0.00827
3.5	0.00289	0.00432
4.0	0.00162	0.00248
4.5	0.000990	0.00153
5.0	0.00064	0.00099

We stress the fact that the above comparison table is only valid for functions which take their maximum values on the real axis.

4.6(c)(ii) The Saddle Point Method

Let us write equation (4.6.10) in the form

$$E_{n+1}(f) = \frac{1}{2\pi i}\int_C h(z)\, \exp[\chi(z)].\, f(z)\, dz \tag{4.6.19}$$

where

$$(4.6.20) \qquad h(z) = \frac{-4\,(2\pi)^{1/2}}{n^{3/2}\left[\log n^2+\pi^2\right]} \cdot \left\{ z\left[1-(-1)^n\right] + 1+(-1)^n \right\}$$

and

$$(4.6.21) \qquad \chi(z) = -\tfrac{3}{2}\log(z^2-1) - \frac{n}{2}\left[(z+1)\log(z+1)-(z-1)\log(z-1)-\log 2\right] + \log f(z) \; .$$

Then the saddle points are the solution of the equation

$$(4.6.22) \qquad \frac{f'(z)}{f(z)} = \frac{n}{2}\log\left(\frac{z+1}{z-1}\right) - \frac{3z}{z^2-1} \; .$$

We may now use the expression (4.2.19) to determine asymptotically the contribution from that part of the contour in the neighbourhood of the saddle points.

Example: Let us take $f(z) = \exp(2z)$. Then from equation (4.6.22) the saddle points are the solutions of the equation

$$(4.6.23) \qquad 2 = \frac{n}{2}\log\left(\frac{z+1}{z-1}\right) - \frac{3z}{3z^2-1} \; .$$

To find an exact solution of equation (4.6.23) is extremely difficult. However an approximate solution is quite sufficient.

Suppose $|Z| \gg 1$ and expand each term in powers of Z^{-1}. Neglecting terms of $O\left(\frac{1}{Z^3}\right)$ we obtain the approximate solution

$$Z = \frac{n+3}{2} \quad . \tag{4.6.24}$$

Equation (4.6.24) confirms our initial assumption that $|Z| \gg 1$.

In this case we also find

$$\chi''(z) = \frac{n(z^2-1) + 3z^2 + 3}{(z^2-1)^2} \tag{4.6.25}$$

$$\sim \frac{n}{z^2-1}\left[\frac{(n+3)\,z^2}{n(z^2-1)}\right], \quad n \text{ large}.$$

From equations (4.2.20) and (4.6.25) we see that $\alpha = i$. Finally the expression (4.2.19) gives us the estimate

$$E_{n+1}(f) = \frac{-4\{\zeta[1-(-1)^n] + 1+(-1)^n\}}{n^2[(\log n)^2+\pi^2]}\left[\frac{n(\zeta^2-1)}{(n+3)\zeta^2}\right]^{1/2} \times \tag{4.6.26}$$

$$\times \exp\left\{2\zeta - \frac{n}{2}\left[(\zeta+1)\log(\zeta+1) - (\zeta-1)\log(\zeta-1) - 2\log 2\right]\right\}$$

where $\zeta = (n+3)/2$.

We compare the actual remainder term with the estimates obtained from equation (4.6.26) in Table 4.6.4.

TABLE 4.6.4

Actual and estimated values and upper bounds of the remainder term in the numerical integration of $\int_{-1}^{1} e^{2x}dx$ using Newton-Cotes quadrature formulae

n	Actual $R_{n+1}(f)$	Asymptotic Estimate	Upper Bound (a/ρ)	
2	-0.215	-0.286	2.12	(2.0)
4	-0.(2)487	-0.(2)557	0.(1)443	(3.0)
6	-0.(4)93	-0.(3)119	C.(3)882	(4.0)
8	-0.(5)1	-0.(5)17	0.(4)14	(5.0)

4.7 Extension to Other Rules

Our applications of the general method described in Section 4.2 have been confined to only a few of the more well-known quadrature rules.

To extend the analysis to other rules we must first obtain suitable asymptotic expressions for the ratio $\psi(z)/\varphi(z)$ Many of these asymptotic forms are not too difficult to obtain.

For example, consider the Radau quadrature formula where the end point -1 of the interval of integration is a fixed abscissa, see Hildebrand [1, p.328] . The function $\varphi(z)$ is given by ([1, equation (8.11.7)])

$$\varphi(z) = P_n^{(0,0)}(z) + P_{n+1}^{(0,0)}(z) \tag{4.7.1}$$

$$= (1+z)\; P_n^{(0,1)}(z)$$

where $P_n^{(\alpha,\beta)}(z)$ is the Jacobi polynomial. Furthermore from Corollary 1 we see that

$$\psi(z) = \int_{-1}^{1} \frac{(1+x)\; P_n^{(0,1)}(x)}{z - x}\, dx \tag{4.7.2}$$

$$= \Pi_{n+1}^{(0,1)}(z) \quad .$$

The functions $\varphi(z)$ and $\psi(z)$ are then known in terms of the Jacobi functions considered in Section 4.3 of this Chapter. Thus we can find asymptotic expressions for these functions.

A list of asymptotic forms for the ratio $\psi(z)/\varphi(z)$ for several quadrature rules is given in Appendix A.

4.8 The Repeated Trapezoidal Rule

We should not leave this Chapter without referring to the repeated trapezoidal rule.

In this case the expression in terms of elementary functions for $\psi(z)/\varphi(z)$ is exact. We recall that for a finite interval of integration the plane for the function $\psi(z)$ is cut along the whole real axis and $\varphi(z)$ has zeros outside the interval of integration. These singularities of the ratio $\psi(z)/\varphi(z)$ must be considered in any deformation of the contours C^+ and C^-.

The trapezoidal rule has been discussed in some detail in Section 2.7 and we shall consider it no further here.

Summary

In this Chapter we have discussed the approximate evaluation of the contour integral form of the remainder term $R_{n+1}(f)$ for large values of n. Making use of known asymptotic estimates for the ratio $\psi(z)/\varphi(z)$ for some of the more common integration formulae it was found that our main concern was the estimation of the quantity $E_{n+1}(f)$ defined by equation (4.1.3).

In some cases these asymptotic expressions are difficult to handle and it is found that further approximations are necessary to make the analysis reasonably simple. In other cases suitable asymptotic expressions are yet to be found; for example, in the Newton-Cotes quadrature formulae we have yet to find an asymptotic expression which we can use when the function has a branch point at an end point of the range.

Nevertheless in those cases which we have considered the methods give fairly accurate estimates of the remainder.

CHAPTER V

CONCLUSION

5.1 Introduction

In Chapter IV we obtained estimates for the remainder term in only a few of the more widely known quadrature rules. Many questions remain to be answered not only on the quadrature rules that we have discussed, but also on those which we have not even considered.

We have, however, set out a method of attack for making estimates of the remainder term in a general quadrature formula. The main task is then to obtain the correct asymptotic expression to use in the conditions pertaining to the particular problem. In the cases we have discussed the asymptotic expressions have been either known or derived, and reasonable estimates of the remainder terms were obtained from them. However, even in these formulae, certain asymptotic expressions have yet to be found; see, for example, the discussion on the Newton-Cotes formulae, Section 4.

To extend the method to other formulae we of course require a knowledge of the asymptotic form of the ratio $\psi(z)/\phi(z)$ for large values of n. Many of these asymptotic forms will no doubt be readily obtained from the existing literature, but others are still to be derived.

In the case of the Gaussian quadrature formulae, it is rather fortunate that the functions $\phi(z)$ and $\psi(z)$ obey several relations; for example, $\phi(z)$ and $\psi(z)$ satisfy three term recurrence relations and second order differential equations. These relations are extremely useful in an investigation of asymptotic forms of these functions, see Elliott and Robinson [41] and [42].

In many formulae, however, the properties of the functions $\phi(z)$ and $\psi(z)$ do not appear to be of much use in an investigation of their asymptotic behaviour. One such formula which has been the subject of recent investigations is Romberg's (see Bauer et al [45]). In Section 2 of this chapter we will discuss this formula in some detail and obtain an expression in terms of a contour integral for the remainder term. As yet we have not been able to obtain a suitable 'simple' asymptotic expression for the remainder term and we defer this problem for future research.

In writing this thesis, it was found that several areas of research were still to be explored. We shall consider two such areas in this chapter.

Firstly, in Section 3 we will consider how new formulae may be obtained from the fundamental theorem and its corollary. We shall in fact obtain a formula which we shall term the Gauss-Whittaker formula. Special cases of this formula are the formulae of Gauss-Hermite, Gauss-Laguerre and Gauss-Bessel (Barrett [19]) and the repeated trapezoidal rule.

In Section 4 we shall discuss what was our original topic, 'A unifying approach to the quadrature of analytic functions over a real interval'. We shall also consider how this idea may be taken one step further to the consideration of integrals along smooth arcs in the complex plane.

5.2 Romberg Integration

The general Romberg integration formula is simply a linear combination of repeated trapezoidal rules. As such, the remainder term may be expressed as a linear combination of the remainder term in the repeated trapezoidal rule. We have discussed in some detail in Section 2.4 of Chapter II a contour integral expression for this remainder and the corresponding expression for Romberg's formula is then not difficult to obtain.

Let us take the interval $[a, b]$ where a and b are abscissae and let us divide the interval into n equal parts. From equation (2.4.47) the repeated trapezoidal rule may be written in the form

$$(5.2.1)\quad \int_a^b f(x)\,dx = \frac{b-a}{n}\sum_{k=0}^{n}{}'' f\left[a+\frac{k(b-a)}{n}\right] + R_{n+1}^{(0)}(f).$$

From equation (2.4.41) and equation (2.4.46) with $\lambda = 0$ and $\nu = n\pi/(b-a)$ the remainder term which we denote by $R_{n+1}^{(0)}(f)$ may be expressed in the form

$$(5.2.2)\quad R_{n+1}^{(0)}(f) = -\frac{1}{2i}\int_C \frac{e^{\pm i\left[\frac{z-a}{b-a}\right]n\pi}}{\sin\left[\frac{z-a}{b-a}\cdot n\pi\right]} f(z)\,dz$$

where the contour C may be chosen as the rectangular contour depicted in Fig. 2.4. In equation (5.2.2) the positive sign is taken in the upper half plane while the negative sign is taken in the lower half plane.

Let us now halve the tabular interval, $(b-a)/n$. Then the remainder term in the repeated trapezoidal rule with $(2n+1)$ points is given by

$$(5.2.3)\quad R_{2n+1}^{(0)}(f) = -\frac{1}{2i}\int_C \frac{e^{\pm i\left[\frac{(z-a)}{b-a}\right]2n\pi}}{\sin\left[\frac{z-a}{b-a}\cdot 2n\pi\right]} f(z)\,dz\ .$$

If we denote by $T_n^{(0)}$ the quadrature sum on the right of equation (5.2.1) then the quadrature sum of the next higher order

Romberg formula is given by

$$(5.2.4) \qquad T^{(1)}(2n) = \frac{4\,T^{(0)}(2n) - T^{(0)}(n)}{3} .$$

This last quadrature sum may be termed as a repeated Simpson's rule. Using the same linear combination as in equation (5.2.4) the remainder term from equations (5.2.2) and (5.2.3) in the repeated Simpson's rule may be written

$$(5.2.5) \qquad \left\{ \begin{aligned} R^{(1)}_{2n+1}(f) &= \frac{4\,R^{(0)}_{2n+1}(f) - R^{(0)}_{n+1}(f)}{3} \\ &= -\frac{1}{6i}\int_C \left[\frac{4e^{\pm\left[\frac{z-a}{b-a}\right]2n\pi i}}{\sin\left[\frac{z-a}{b-a}\cdot 2n\pi\right]} - \frac{e^{\pm\left[\frac{z-a}{b-a}\right]n\pi i}}{\sin\left[\frac{z-a}{b-a}\cdot n\pi\right]} \right] f(z)\,dz. \end{aligned} \right.$$

The general Romberg formula is obtained from repeated bisection of the tabular interval. In fact, the general quadrature sum is obtained from the recurrence relation

$$(5.2.6) \qquad T^{(m)}(2^m n) = \frac{4^m\,T^{(m-1)}(2^m n) - T^{(m-1)}(2^{m-1} n)}{4^m - 1} .$$

Thus the general expression for the remainder term may be obtained from the recurrence relation

$$(5.2.7) \qquad R^{(m)}_{2^m n+1}(f) = \frac{4^m\,R^{(m-1)}_{2^m n+1}(f) - R^{(m-1)}_{2^{m-1} n+1}(f)}{4^m - 1}$$

where $R^{(0)}_{n+1}(f)$ is given by equation (5.2.2).

From the recurrence relation (5.2.7) we can obtain an expression for the remainder in terms of a contour integral for the general quadrature formula. The integrand in the contour integral is rather unwieldy, and at present we have been unable to obtain a simple form for the ratio $\psi(z)/\phi(z)$ for large values of $2^m . n$.

The Generalised Romberg Formula

Romberg's formulae have been generalised by choosing subdivisions other than bisections by Bulirsch [46] . Bulirsch obtained an expression for the remainder term of the formula in terms of a high order derivative.

Since this generalised formula is again a linear combination of repeated trapezoidal rules, it is not difficult to obtain a contour integral expression for the remainder in terms of a recurrence relation similar to equation (5.2.7). An analysis of this remainder term appears to be even more difficult.

In fact, in all the repeated rules, excepting the special case of the repeated trapezoidal rule, the expressions for $\psi(z)/\phi(z)$ have proved too difficult to handle. It is hoped that this problem will be overcome in the near future.

We shall discuss another possible approach to this problem in the following Section.

5.3 New Formulae

On examination of the fundamental theorem of Chapter II, it appears that to obtain a quadrature rule we need only find functions $\psi(z)$ and $\phi(z)$ which satisfy the conditions of that theorem. On the other hand it may be more convenient to choose $\phi(z)$ first to have zeros at certain points of the interval of integration and generate $\psi(z)$ from the corollary of the theorem. We could in fact choose $\psi(z)$ to take the more general form given by equation (1.2.15).

We recall that if $\phi(z)$ is a function of z which has zeros at the abscissae of the quadrature formula then the function $\psi(z)$ satisfying the conditions of the fundamental theorem and its corollary is given by

$$(5.3.1) \qquad \psi(z) = \int_a^b \frac{\omega(x)\,\phi(x)\,dx}{z-x} \quad .$$

More generally we could, according to equation (1.2.15), choose, in order to generate a quadrature formula, a function $\psi^{x}(z)$ defined by

$$(5.3.2) \qquad \psi^{x}(z) = \psi(z) + p(z)$$

where $\mathcal{P}(z)$ is an arbitrary function of z analytic in the finite part of the complex plane.

In restricting ourselves to equation (5.3.1) the weight factors $\lambda_{k,n}$, $k = 0(1)n$, are determined for us by the fundamental theorem once the zeros $x_{k,n}$, $k = 0(1)n$, have been prescribed. In fact from equation (1.2.9) we have

$$(5.3.3) \qquad \lambda_{k,n} = -\frac{\psi(x_{k,n})}{\varphi'(x_{k,n})}, \quad k = 0(1)n.$$

If, however, we take the more general form, equation (5.3.2), we can perhaps choose $\mathcal{P}(z)$ to satisfy certain other prescribed conditions on the quadrature rule. We may, for example, wish to prescribe the weight factors.

As an example let us take a formula in which the zeros are at the points $x_{k,n}$, $k = 0(1)n$, and the weight factors are $\lambda^{\times}_{k,n}$, $k = 0(1)n$. Then from the equation (1.2.9) we have

$$(5.3.4) \qquad \lambda^{\times}_{k,n} = -\frac{\psi^{\times}(x_{k,n})}{\varphi'(x_{k,n})}, \quad k = 0(1)n.$$

From equations (5.3.2) and (5.3.4) we see that the function $\mathcal{P}(z)$ must satisfy the $(n+1)$ conditions

(5.3.5) $$\mathcal{P}(x_{k,n}) = (\lambda_{k,n} - \lambda^{x}_{k,n})\,\phi'(x_{k,n}), \quad k = 0(1)n.$$

Therefore if we choose $\mathcal{P}(z)$ to be a polynomial of degree n of the form $a_n z^n + a_{n-1} z^{n-1} + \cdots + a_0$ the set of equations (5.3.5) will give us $(n+1)$ equations for the coefficients $a_n, a_{n-1}, \cdots, a_0$.

This attack may provide us with an answer to the problem of the previous Section.

Let us take the simplest case of the repeated trapezoidal rule over $[-1, 1]$ with three abscissae at -1, 0 and 1 with weight factors $\frac{1}{2}$, 1 and $\frac{1}{2}$ respectively. Then rather than, as was previously done, choose $\phi(z) = \sin \pi z$ let us take $\phi(z)$ to be the polynomial

(5.3.6) $$p_3(z) = (z-1)\, z\, (z+1) .$$

The function $p_3(z)$ is of course the polynomial discussed in the case of the Newton-Cotes formula (Simpson's rule) and the corresponding function $\psi(z)$ we have denoted by $q_3(z)$.

Since we are prescribing three weight factors we take $\mathcal{P}(z)$ to be a polynomial of degree 2.

Thus from equation (5.3.2) we have

(5.3.7) $$\psi^{x}(z) = q_3(z) + a_2 z^2 + a_1 z + a_0 .$$

The coefficients a_2, a_1 and a_0 are chosen to satisfy equations (5.3.5) and we have

$$(5.3.8)\quad \begin{cases} a_2 + a_1 + a_0 = -1/3 , \\ a_2 - a_1 + a_0 = -1/3 , \\ a_0 = -1/3 \end{cases}$$

where we have used the fact that the weight factors for Simpson's rule are $1/3$, $4/3$ and $1/3$.

From equations (5.3.8) we see that $a_2 = a_1 = 0$ and $a_0 = -1/3$. We would therefore choose for this particular rule

$$(5.3.9)\quad \begin{cases} \phi(z) = p_3(z) , \\ \psi(z) = q_3(z) - 1/3 . \end{cases}$$

For the repeated trapezoidal rule with 4 points in $[-1, 1]$ we would take $\phi(z) = p_4(z)$ and find $\psi(z) = q_4(z) + 4z/27$.

Proceeding in this way we may be able to determine the appropriate function $\psi(z)$ to use in the general Romberg formula.

Furthermore these ideas may be used to obtain new quadrature formulae. The method has the added advantage as far as we are concerned of having the remainder term in terms of a contour integral.

We shall in this Section consider a formula obtained from consideration of the confluent hypergeometric function and discuss some special cases of it.

5.3(a) The Gauss-Whittaker Quadrature Rule

The rules which we shall consider in this Section are relevant to either the semi-infinite or doubly-infinite intervals of integration.

Let us consider first the interval $(0, \infty)$ and choose $\omega(z)$ and $\phi(z)$ as follows:

$$\omega(z) = e^{-z} z^{c+r-1} \tag{5.3.10}$$

and

$$\phi(z) = \frac{\Gamma(1-a)\,\Gamma(c)}{\Gamma(c-a)}\, {}_1F_1(a, c; z) \tag{5.3.11}$$

where ${}_1F_1$ is the confluent hypergeometric function of the first kind.

From Corollary 1, equation (1.2.14), we have

$$\psi(z) = \int_0^\infty \frac{\omega(x)\,\phi(x)}{z-x}\, dx \tag{5.3.12}$$

provided the integral on the the right exists. Now from Erdélyi et al [33, p.385] we have on substituting equations (5.3.10) and (5.3.11) into equation (5.3.12)

$$(5.3.13) \qquad \psi(z) = \frac{[\Gamma(1-a)\,\Gamma(c)]^2}{\Gamma(c-a)} \cdot (-z)^c z^{r-1}\, U(c-a, c; -z)$$

where $|\arg(-z)| < \pi$, $-\mathcal{R}\ell(c) < r < 1 - \mathcal{R}\ell(a)$, for $r = 0, 1, 2, \ldots$, and $U(c-a, c; -z)$ is the confluent hypergeometric function of the second kind.

Alternatively the functions $\psi(z)$ and $\varphi(z)$ may have been obtained directly from the fundamental theorem. For, from Slater [43, p.21] we have, in $0 < x < \infty$,

$$(5.3.14) \begin{cases} \Gamma(1-a)\,\Gamma(c)\, x^{c+r-1}\left[e^{\pi i c} U(c-a, c; xe^{\pi i}) - e^{-\pi i c} U(c-a, c; xe^{-\pi i})\right] \\ \qquad = 2\pi i\, e^{-x} x^{c+r-1}\, {}_1F_1(a, c; x) \end{cases} .$$

In equation (5.3.14) there does not appear to be any restrictions on a, c similar to those in equation (5.3.13).

In terms of the Whittaker functions $M_{k,m}(z)$, $W_{k,m}(z)$ we have on putting $a = \frac{1}{2} + m - k$, $c = 1 + 2m$ and $r = 0$ in equations (5.3.10), (5.3.11) and (5.3.13), (see Slater 43, p. 13),

$$(5.3.15) \qquad \omega(z) = e^{-z} z^{2m} ,$$

(5.3.16) $$\phi(z) = e^{\frac{1}{2}z} z^{-m-\frac{1}{2}} M_{k,m}(z)$$

and

(5.3.17) $$\psi(z) = \Gamma(k-m+\tfrac{1}{2})\,\Gamma(2m+1)\, e^{\frac{1}{2}z} (-z)^{m+k-\frac{1}{2}} W_{-k,m}(-z) .$$

The last three functions satisfy the conditions of the fundamental theorem and determine for us a quadrature rule which we shall term as the 'Gauss-Whittaker' quadrature formula.

The abscissae of the formula are those zeros of $M_{k,m}(z)$ which lie on the interval $(0, \infty)$ and the weights are given by equation (1.2.9) of Chapter I.

Discussions of the zeros of $M_{k,m}(z)$ are to be found in Slater [43, p. 102] and Erdélyi et al [47, p. 288]. Of interest to us are the cases where zeros do exist in $(0, \infty)$.

We mention two such cases.

<u>Case (i)</u>: Suppose k and m are both real and that $m > -\frac{1}{2}$. Then if we write $k = p + m + \frac{1}{2} - \theta,\ 0 < \theta \leq 1,\ M_{k,m}(z)$ has p positive (real) zeros.

<u>Case (ii)</u>: If k, m are real and $m = -\frac{1+q}{2} + \theta^{x},\ 0 < \theta^{x} < 1$ then $M_{k,m}(z)$ has $p-q$ real positive zeros where $k = p + m + \frac{1}{2} - \theta,\ 0 < \theta < 1$.

In the latter case the function $M_{k,m}(z)$ has zeros lying outside the basic interval ($0, \infty$) and any deformation of the contours C^+, C^- in the expression for the remainder term would have to take these zeros into consideration.

The remainder term of the 'Gauss-Whittaker' formula is given immediately by equation (1.2.2) of the fundamental theorem. Our first aim as far as estimating the remainder term is concerned is finding asymptotic expressions for the ratio $\psi(z)/\phi(z)$ in this case for large values of k .

Suitable expressions are to be found in Slater [43, Chapt.4] .

There are three important expressions which should be considered depending on whether $|z/4k|$ is small, $|z/4k|$ is large or $z \sim 4k$.

A fuller investigation of this formula and its remainder term we defer to a later date.

Some Special Cases

The general expressions (5.3.10), (5.3.11) and (5.3.13) with appropriate choices of the constants, a, C and r , give rise to many familiar formulae and two formulae which, as far as we know, have not appeared previously in the literature. It is more convenient to obtain these special cases in terms of the confluent hypergeometric functions than the Whittaker functions.

Since the asymptotic expressions for the confluent hypergeometric functions are well known the relationship of these special cases with these functions is useful (in conjunction with Chapter IV) for making estimates of the remainder term in the corresponding quadrature rules.

The Gauss-Laguerre Formula

Taking $\tau = 0$ and putting $a = -n$, $c = \alpha + 1$ in equations (5.3.10), (5.3.11) and (5.3.13) we have, see Slater [47, p. 95]

$$(5.3.18) \quad \begin{cases} \omega(z) = e^{-z} z^{\alpha}, \\ \phi(z) = \dfrac{\Gamma(n+1)\,\Gamma(\alpha+1)}{\Gamma(\alpha+n+1)}\; {}_1F_1(-n, \alpha+1; z) = L_n^{(\alpha)}(z), \\ \psi(z) = \dfrac{\left[\Gamma(n+1)\,\Gamma(\alpha+1)\right]^2}{\Gamma(\alpha+n+1)}\, e^{\pi i(\alpha+1)} z^{\alpha}\, U(\alpha+n+1, \alpha+1, -z) = \Lambda_n^{(\alpha)}(z) . \end{cases}$$

Equations (5.3.18) are the functions considered in the discussion of the Gauss-Laguerre quadrature rule in Section 2.4(a).

The Gauss-Bessel Formula

The conditions imposed by the theorem on the functions $\phi(z)$

and $\psi(z)$ are obviously unaltered by multiplying each of these functions by a constant or in fact by any function of z which does not have a singularity on the interval of integration.

Let us now put $a = (c-a)$ and choose

$$\omega(z) = e^{-z}\left(\frac{4a}{K}z\right)^{c-1} \tag{5.3.19}$$

and

$$\varphi(z) = \left(\frac{K^{1/2}}{2}\right)^{c-1}\frac{1}{\Gamma(c)}\,{}_1F_1(c-a, c; z) \tag{5.3.20}$$

where K is a positive real constant. To satisfy the conditions (5.3.14) we must then have

$$\psi(z) = -\Gamma(1+a-c)\left(\frac{K}{2}\right)^{1/2}\left(\frac{4a}{K}\right)^{c-1}(-z)^{c-1}\,U(a, c; -z)\,. \tag{5.3.21}$$

Now suppose a is real and let us replace z by $Kz/4a$ in equations (5.3.19), (5.3.20) and (5.3.21). We obtain

$$\left\{\begin{aligned} \overset{*}{\omega}(z) &= e^{-K/4a\, z}\, z^{c-1}\,, \\ \overset{*}{\varphi}(z) &= \left(\frac{K}{2}^{1/2}\right)^{c-1}\frac{1}{\Gamma(c)}\,{}_1F_1\left(c-a, c; \frac{-\frac{K}{4}z}{a}\right)\,, \\ \overset{*}{\psi}(z) &= -\Gamma(1+a-c)\left(\frac{K^{1/2}}{2}\right)^{c-1}(-z)^{c-1}\,U\left(a, c; \frac{-\frac{K}{4}z}{a}\right)\,. \end{aligned}\right. \tag{5.3.22}$$

Letting a tend to infinity equations (5.3.22), from Slater [43, p.67] , become

$$(5.3.23)\quad \begin{cases} \overset{\times}{\omega}(z) = z^{\alpha}, \\ \overset{\times}{\varphi}(z) = z^{-\alpha/2} J_{\alpha}[(Kz)^{1/2}], \\ \overset{\times}{\psi}(z) = -2(-z)^{\alpha/2} K_{\alpha}[(Kz)^{1/2}] \end{cases}$$

where $\alpha = c-1$.

These are of course the functions relevant to the Gauss-Bessel formula discussed in Section 2.4(a).

A Simple Formula

The equations (5.3.23) take a particularly simple form if we choose $\alpha = 1/2$. We then find on making use of the expressions for the Bessel functions in terms of circular functions and multiplying through by a constant factor

$$(5.3.24)\quad \begin{cases} \overset{\times}{\omega}(z) = z^{1/2}, \\ \overset{\times}{\varphi}(z) = z^{-1/2} \sin(Kz)^{1/2}, \\ \overset{\times}{\psi}(z) = -\pi e^{i(Kz)^{1/2}}. \end{cases}$$

Equations (5.3.24) provide a rather simple formula not unlike, in form, the repeated trapezoidal rule. The formula may be written

$$(5.3.25) \quad \int_0^\infty z^{\frac{1}{2}} f(x)\, dx = 2\left(\frac{\pi}{K^{\frac{1}{2}}}\right)^3 \sum_{r=1}^{\infty} r^2 f\left(\frac{r^2\pi^2}{K}\right) + R(f).$$

A comparison of this formula with the repeated trapezoidal rule over $(-\infty, \infty)$ suggests that this is the corresponding rule to use when the interval is $(0, \infty)$. Although further investigation is necessary it would appear that this formula may provide accurate results in certain cases corresponding to those attained by using the repeated trapezoidal rule over $(-\infty, \infty)$, see Goodwin [14] .

The Gauss-Hermite Formula

Let us now take $c = \frac{1}{2}, a = -m$ and $r = 0$. Then equations (5.3.10), (5.3.11) and (5.3.13) become

$$(5.3.26) \quad \begin{cases} \omega(z) = e^{-z} z^{-\frac{1}{2}}, \\ \phi(z) = (-1)^m \dfrac{(2m)!}{m!}\, {}_1F_1\left(-m, \tfrac{1}{2}; z\right), \\ \psi(z) = (-1)^m (2m)!\, \Gamma(\tfrac{1}{2})\, (-z)^{\frac{1}{2}}\, U\left(\tfrac{1}{2}+m, \tfrac{1}{2}; -z\right). \end{cases}$$

We now transform to the plane of the complex variable ζ where $z = \zeta^2$. Thus the interval ($0, \infty$) in the z-plane corresponds to the interval ($-\infty, \infty$) in the ζ-plane. Equations (5.3.26) are then related to a quadrature rule over ($-\infty, \infty$). We have on multiplying through by ζ, (see Slater [43, p.99])

$$
(5.3.27) \quad \begin{cases} \omega(\zeta) & = e^{-\zeta^2}, \\ \varphi(\zeta) & = (-1)^m \dfrac{(2m)!}{m!} \, {}_1F_1(-m, \tfrac{1}{2}; \zeta^2) \quad = H_{2m}(\zeta), \\ \psi(\zeta) & = (-1)^{m+\frac{1}{2}} \Gamma(\tfrac{1}{2})(2m)! \, U(\tfrac{1}{2}+m, \tfrac{1}{2}, -\zeta^2) = \eta_{2m}(\zeta). \end{cases}
$$

The functions are those used in the Gauss-Hermite formula Section 2.4) with an even number of ordinates. The corresponding expressions for the 'odd' formula are obtained by taking $c = 3/2$, $a = -m$. We find

$$
(5.3.28) \quad \begin{cases} H_{2m+1}(\zeta) & = (-1)^m (2m+1)! \; 2\zeta \, {}_1F_1(-m, \tfrac{3}{2}; \zeta^2), \\ \\ \eta_{2m+1}(\zeta) & = (-1)^{m+\frac{3}{2}} (2m+1)! \; \Gamma(\tfrac{1}{2}) \, \zeta \, U(\tfrac{3}{2}+m, \tfrac{3}{2}, -\zeta^2). \end{cases}
$$

The Gauss-Bessel Formula over ($-\infty, \infty$)

Corresponding to the 'Gauss-Bessel' formula, (see Barrett [19]) over $(0, \infty)$, we have a similar type of formula over $(-\infty, \infty)$.

Again let us take our equations in the form of equations (5.3.22),

$$
(5.3.29) \quad \begin{cases}
\omega(z) &= e^{-(K/4a)z} z^{c-1}, \\
\phi(z) &= \left(\frac{K^{1/2}}{2}\right)^{c-1} \frac{1}{\Gamma(c)} {}_1F_1\left(c-a, c; \frac{\frac{K}{4}z}{a}\right), \\
\psi(z) &= -\Gamma(1+a-c)\left(\frac{K^{1/2}}{2}\right)^{c-1}(-z)^{c-1} U\left(a, c; \frac{-\frac{K}{4}z}{a}\right),
\end{cases}
$$

and let us transform to the ζ-plane, $z = \zeta^2$. Proceeding as before to the limit as a tends to infinity equations (5.3.29) become, on multiplying through by a factor ζ,

$$
(5.3.30) \quad \begin{cases}
\omega(\zeta) &= \zeta^{2c-3}, \\
\phi(\zeta) &= \zeta^{2-c} J_{c-1}(K^{1/2}\zeta), \\
\psi(\zeta) &= (e^{\mp i\pi})^{c+1} 2\, \zeta^{c-1} K_{c-1}(K^{1/2}\zeta e^{\mp i\pi/2})
\end{cases}
$$

where the upper signs are to be taken in the upper half-plane and the lower sign in the lower half-plane.

The integration formula corresponding to equation (5.3.30) may be called a 'Gauss-Bessel' formula for $(-\infty, \infty)$.

<u>The Repeated Trapezoidal Rule</u>

It is interesting to note that if we take $c = 3/2$ in over ($0, \infty$), we have a similar type of formula over ($-\infty, \infty$).

Again let us take our equations in the form of equations (5.3.22),

$$
(5.3.29) \quad \begin{cases} \omega(z) &= e^{-(K/4a)z} z^{c-1}, \\ \phi(z) &= \left(\frac{K}{2}^{1/2}\right)^{c-1} \frac{1}{\Gamma(c)} {}_1F_1\left(c-a, c; \frac{\frac{K}{4} z}{a}\right), \\ \psi(z) &= -\Gamma(1+a-c)\left(\frac{K}{2}^{1/2}\right)^{c-1} (-z)^{c-1} U\left(a, c; \frac{-\frac{K}{4} z}{a}\right), \end{cases}
$$

and let us transform to the ζ-plane, $z = \zeta^2$. Proceeding as before to the limit as a tends to infinity equations (5.3.29) become, on multiplying through by a factor ζ,

$$
(5.3.30) \quad \begin{cases} \omega(\zeta) &= \zeta^{2c-3}, \\ \phi(\zeta) &= \zeta^{2-c} J_{c-1}(K^{1/2}\zeta), \\ \psi(\zeta) &= (e^{\mp i\pi})^{c+1} 2\, \zeta^{c-1} K_{c-1}(K^{1/2}\zeta e^{\mp i\pi/2}) \end{cases}
$$

where the upper signs are to be taken in the upper half-plane and the lower sign in the lower half-plane.

The integration formula corresponding to equation (5.3.30) may be called a 'Gauss-Bessel' formula for ($-\infty, \infty$).

The Repeated Trapezoidal Rule

It is interesting to note that if we take $c = 3/2$ in equations (5.3.30) then we have

$$(5.3.31)\quad \begin{cases} \omega(z) = 1 , \\ \varphi(z) = \left(\dfrac{2}{\pi K^{1/2}}\right)^{1/2} \sin (K^{1/2} z) , \\ \psi(z) = -\left(\dfrac{2\pi}{K^{1/2}}\right)^{1/2} e^{\pm i K^{1/2} z} . \end{cases}$$

The equations (5.3.31) were those considered in conjunction with the trapezoidal rule in Section 2.4(c).

It is well known that the application of the repeated trapezoidal rule to the integrals over $(-\infty, \infty)$ yields surprisingly accurate results for many functions, see Goodwin [14] .

From the above derivation this rule appears to be one of a family of quadrature formulae some of which are of Gaussian type. This admits the conjecture that the accuracy of this formula is due in part to the fact that the repeated trapezoidal rule is Gaussian in nature.

5.4 A Unified Treatment of Quadrature Formulae

In the process of obtaining an expression for the remainder term in terms of a contour integral there appears to be a certain unifying treatment of many of the apparently unrelated quadrature formulae. We have for example seen how the Newton-Cotes formulae and the Gauss-type formulae are particular cases of the one theorem.

We have also seen in Section 5.3 how it may be possible to find functions $\psi(z)$ and $\varphi(z)$ for any quadrature formula (with a finite number of abscissae) in which both the abscissae and the weight factors are prescribed.

Since Theorem 1 is a particular case of Theorem 2 all the formulae we have considered in this thesis are particular cases of the one theorem. This provides us with a basis for a unified treatment of quadrature formulae. As far as our subsequent analysis is concerned it is convenient to have the remainder term in the required form of a contour integral.

This unifying idea may be taken even further if we consider integrals along smooth arcs in the complex plane. An expression in terms of a contour integral for the remainder term in such formulae has been obtained by Barnhill [26] for the special case when the function was analytic at all points of the arc including its end points. Our generalisation allows singularities at the end points.

The generalisation of the fundamental theorem is not difficult and we shall not give details here. The corollary of this generalisation corresponding to the corollary of Theorem 1 again comes immediately from results in Muskhelishvili [28] .

5.5 Final Summary

The original task of this thesis was the topic outlined in the previous Section. Subsequent developments lead to a consideration of the remainder term in several of the more widely used quadrature rules for large values of a parameter.

To this end an expression for the remainder term in terms of a contour integral was obtained.

This expression together with known asymptotic forms of the ratio $\psi(z)/\varphi(z)$ was also found useful in discussing the convergence of certain quadrature schemes.

Estimates of the remainder term were then obtained for large values of n using familiar complex variable techniques. It may be argued that the methods require too great a knowledge of mathematical analysis to be universally acceptable, but the estimates are certainly realistic when compared to other techniques which require less mathematical 'sophistication'.

So far we have been more successful with interpolatory quadrature rules (those rules obtained from an integration of a Lagrangian or a Hermite interpolation formula) than with formulae of non-interpolatory type like Romberg's, Section 5.2. However, as we have indicated throughout, many questions remain to be answered and it is hoped that further research will provide an answer to them.

We list in this appendix some of the known asymptotic expressions corresponding to the various quadrature rules and the regions in which they are valid

Integration Formula		Asymptotic Expression for $\psi(z)/\varphi(z)$	Region of Validity
Repeated Trapezoidal Rule		$e^{+i\pi(z-a).\nu/h} / \sin[\pi(z-a).\nu/h]$	$\mathrm{Im}(z) > 0$
		$e^{-i\pi(z-a).\nu/h} / \sin[\pi(z-a).\nu/h]$	$\mathrm{Im}(z) < 0$
Gauss-Jacobi	1.*	$2\pi \cdot \dfrac{(z-1)^{\alpha}(z+1)^{\beta}}{[z+(z^2-1)^{1/2}]^{2n+\alpha+\beta+3}}$	all z except in neighbourhood of $[-1,1]$
	2.	$-2(-z-1)^{\beta}(-z+1)^{\alpha} \cdot \dfrac{K_{\beta}[(2n+\alpha+\beta+3)\xi]}{I_{\beta}[(2n+\alpha+\beta+3)\xi]}, \quad z = -\cosh 2\xi$	z near -1 and not near $+1$
	3.	$2(z+1)^{\beta}(z-1)^{\alpha} \cdot \dfrac{K_{\alpha}[(2n+\alpha+\beta+3)\xi]}{I_{\alpha}[(2n+\alpha+\beta+3)\xi]}, \quad z = \cosh 2\xi$	z near $+1$ and not near -1
Gauss Laguerre	1.†	$-2\pi\left[1+\dfrac{\alpha+1}{2(n+1)}\right]^{\alpha/2-1/4} \cdot e^{-z}(-z)^{\alpha} \cdot \exp\left\{-2\left[\left(n+1+\frac{\alpha+1}{2}\right)^{1/2}+(n+1)^{1/2}\right](-z)^{1/2}\right\}$	z bounded and not in neighbourhood of $(0,\infty)$
	2.	$-2\,e^{-z}(-z)^{\alpha} \cdot \dfrac{K_{\alpha}\{[4(n+1)+2\alpha+2]^{1/2}(-z)^{1/2}\}}{I_{\alpha}\{[4(n+1)+2\alpha+2]^{1/2}(-z)^{1/2}\}}$	z bounded including 0

*The branches of $(z-1)^{\alpha}$ and $(z+1)^{\beta}$ are specified by $|\arg(z-1)| < \pi$ and $|\arg(z+1)| < \pi$.

†The branch of $(-z)^{\alpha}$ is specified by $|\arg(-z)| < \pi$.

Integration Formula	Asymptotic Expression for $\psi(z)/\phi(z)$	Region of Validity
Gauss-Hermite	$2\pi(-1)^n e^{-i\pi/2} e^{-z^2} \cdot \exp\{+2(2n+4)^{1/2} z i\}$	Im(z) > 0
	$2\pi(-1)^n e^{+i\pi/2} e^{-z^2} \cdot \exp\{-2(2n+4)^{1/2} z i\}$	Im(z) < 0
Newton-Cotes (over $[-1,1]$)	$\frac{-4(2\pi)^{1/2}(z^2-1)^{-1/2}}{n^{3/2}[(\log n)^2+\pi^2]}\left[\frac{1}{z-1}-\frac{(-1)^n}{z+1}\right] \times$ $\times \exp\left\{-n\left[\frac{z+1}{2}\log(z+1)-\frac{z-1}{2}\log(z-1)-\log 2\right]\right\}$	all z except in neighbourhood of $[-1,1]$

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